TÉCNICO+
FORMAÇÃO AVANÇADA

Deep Learning

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Program for today

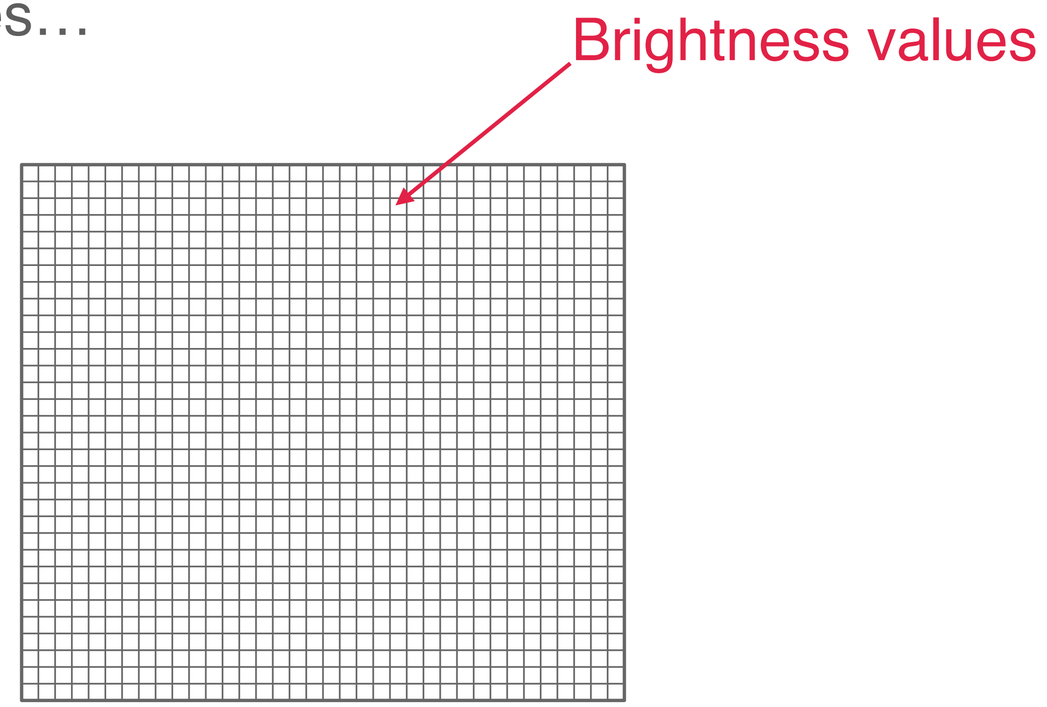
Representations

Recurrent neural networks

GRUs and LSTMs

So far…

- We played around with images…



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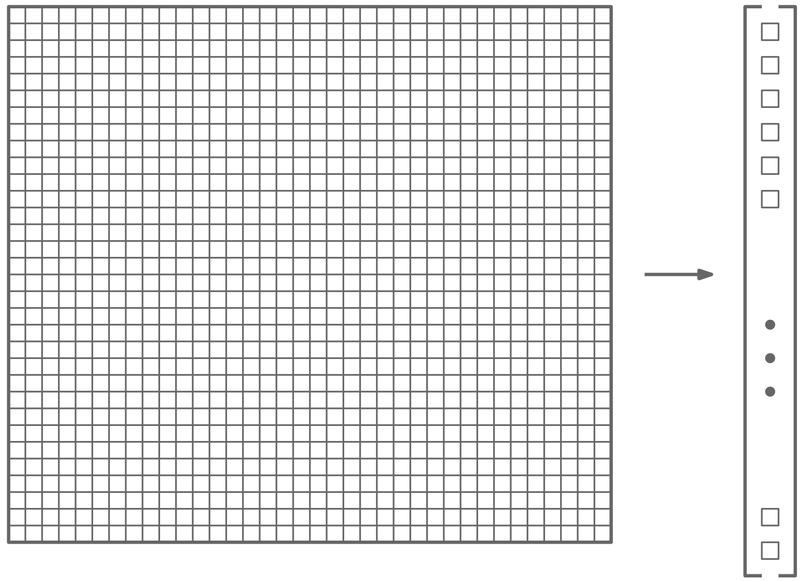

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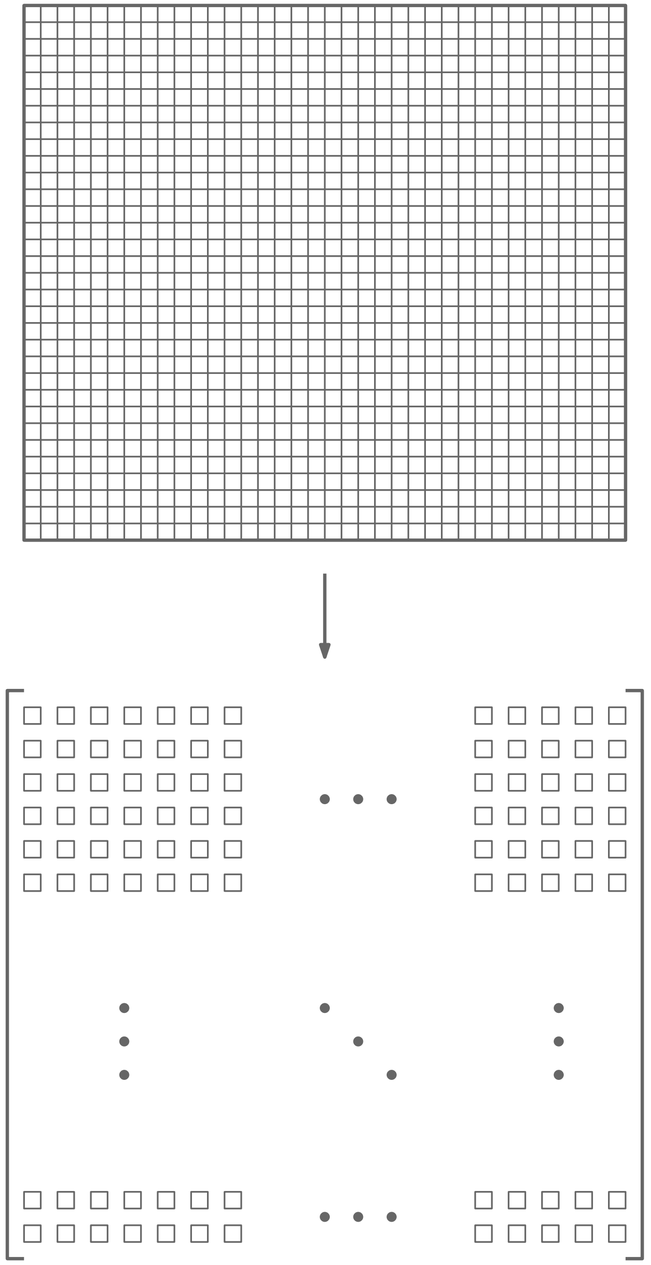
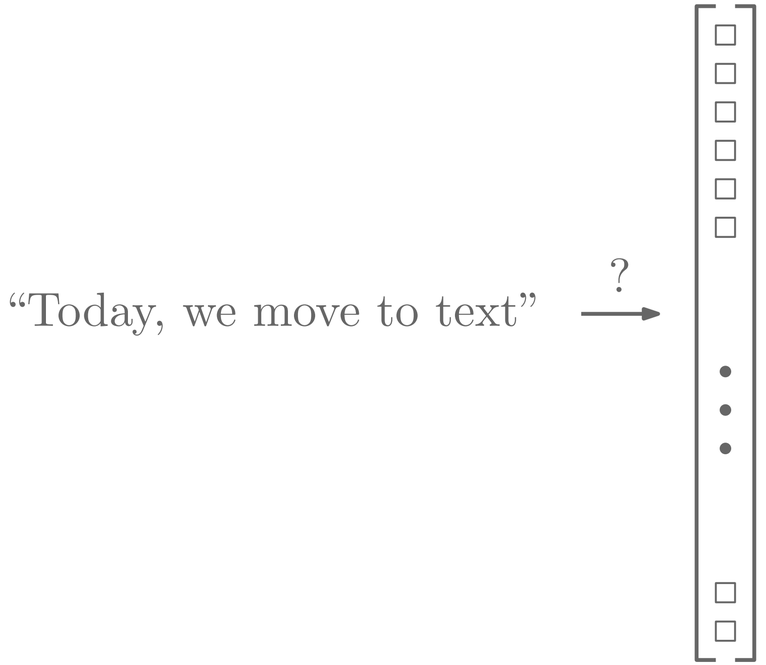


Today, we move to text

Problem n. 1

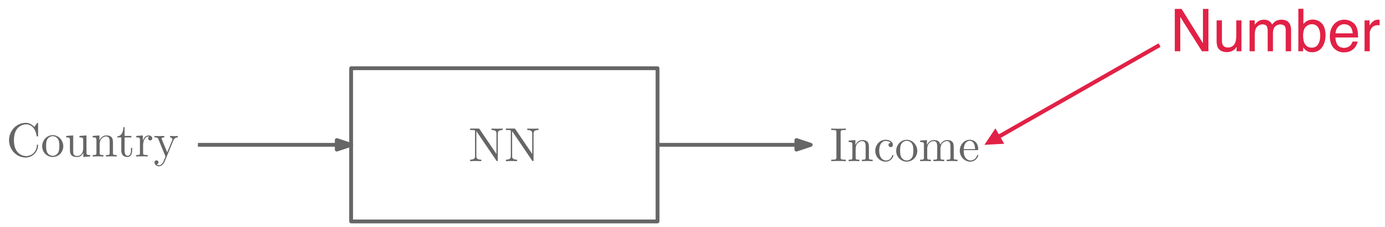
- How do we represent text as a vector/matrix of numbers?



Representations

Representations

- Neural networks expect vectors/matrices of numbers as inputs
- How can we represent a non-numerical quantity as a vector/matrix of numbers?
- E.g.:
  - Suppose we want to predict average income given the country



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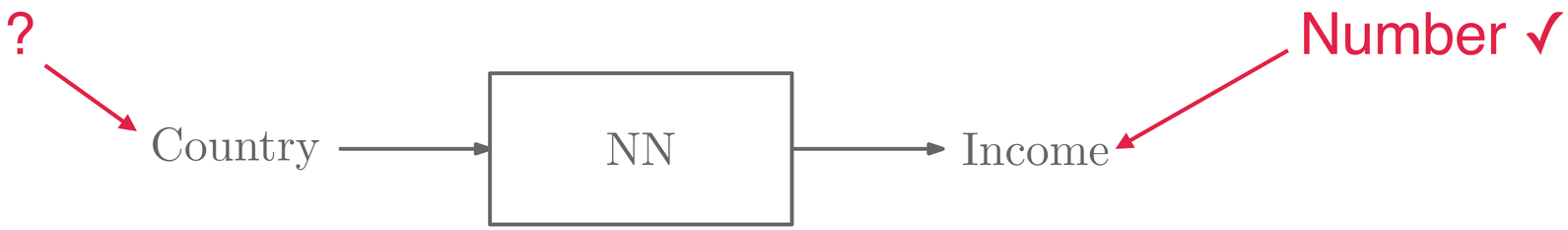


Idea n. 1

- Naive idea:
  - List all *N* countries
  - Assign to each country a number from 1 to *N*

1. Afghanistan
2. Albania
3. Algeria
4. Andorra
5. Angola
6. Antigua and Barbuda
7. Argentina

… …

Problem:

The numbers have no numerical meaning

Idea n. 2

- One-hot encoding
  - List all *N* countries
  - Represent each country as a *N*-element vector with a single 1

Afghanistan

Albania

Algeria

Andorra

Angola

Antigua and Barbuda

Argentina

…

Idea n. 2

One-hot encoding:

We can interpret these numbers as “probabilities”

1	0	0	0	0	0	0	…	0
0	1	0	0	0	0	0	…	0
0	0	1	0	0	0	0	…	0
0	0	0	1	0	0	0	…	0
0	0	0	0	1	0	0	…	0
0	0	0	0	0	1	0	…	0
0	0	0	0	0	0	1	…	0
…	…	…	…	…	…	…	…	…

Afghanistan

Albania

Algeria

Andorra

Angola

Antigua and Barbuda

Argentina

…

What about text?

- List all possible words in our vocabulary
- Represent each word using one-hot encoding

One-hot encoding

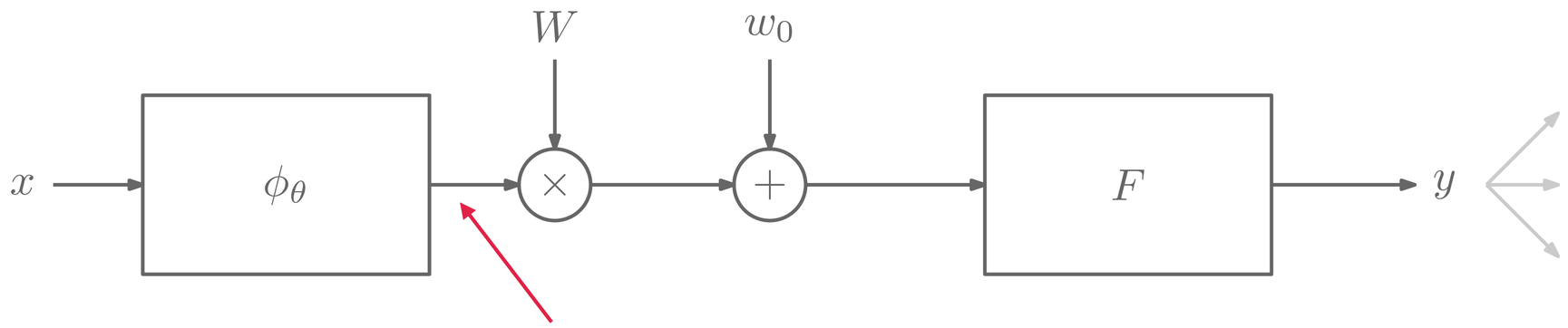
- Works fine for text
- However…
  - One-hot encoding may lead to very large representations

    (1,000,000 words → 1,000,000 element vector)
  - Representations are local (one dimension per word)

Can we do better?

Learning representations

- Neural networks are good at learning representations

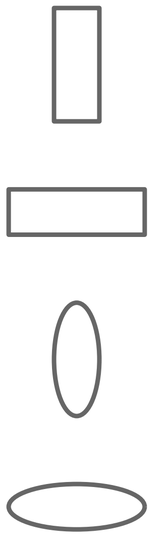


Learning representations

- Neural networks are good at learning representations
- We can try to learn a better (non-local) representation for our input

Local vs distributed representations

No pattern



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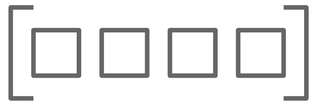
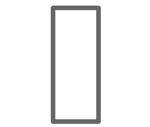
No pattern 



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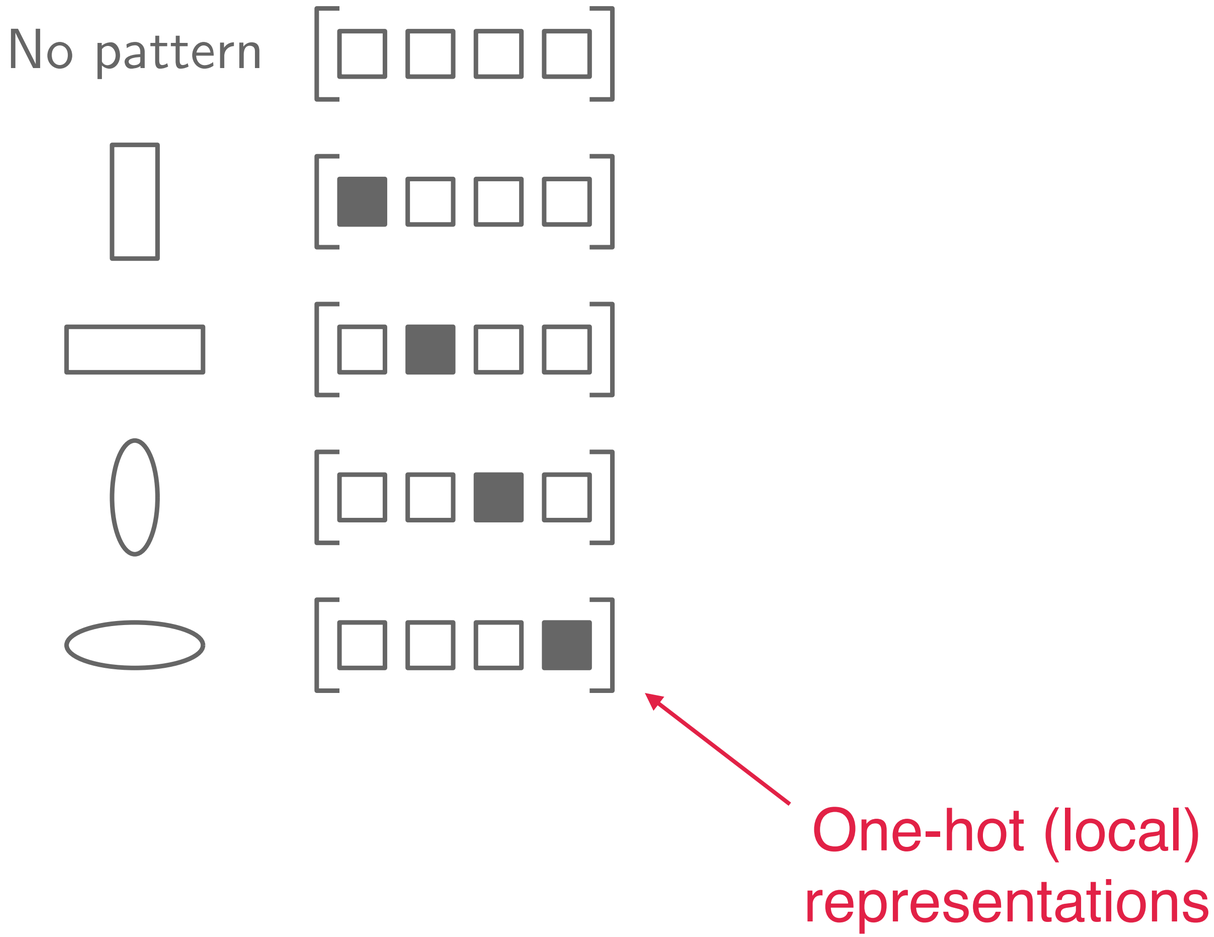

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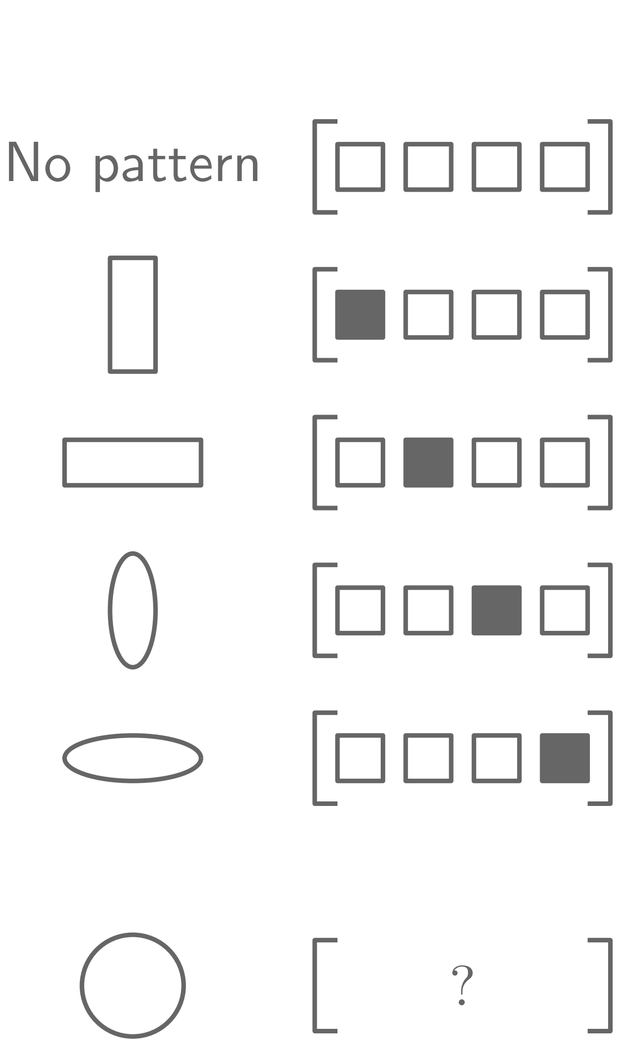

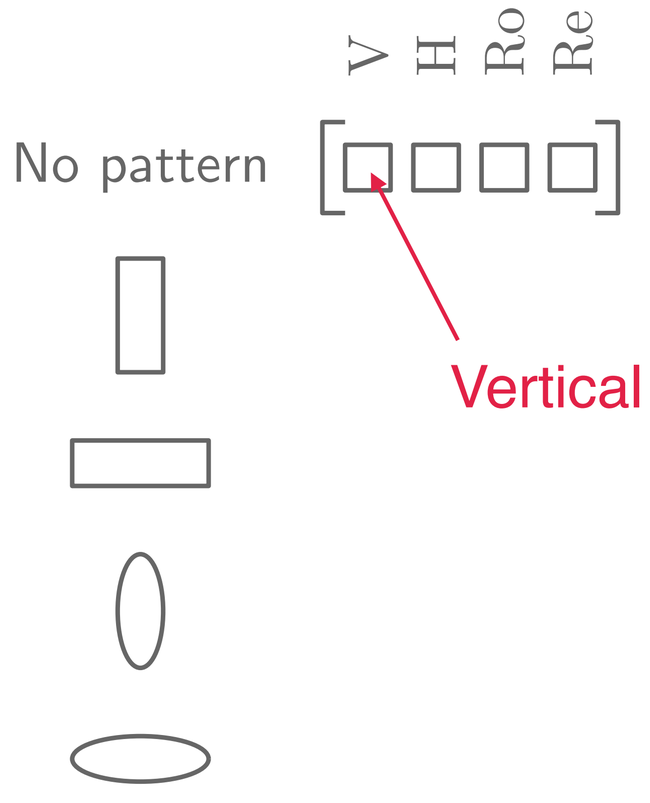

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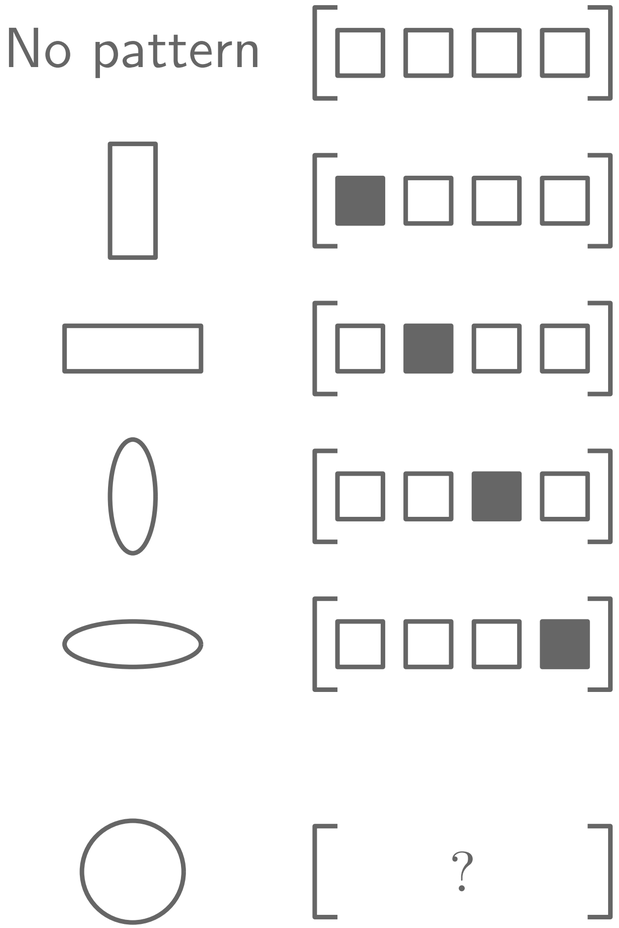

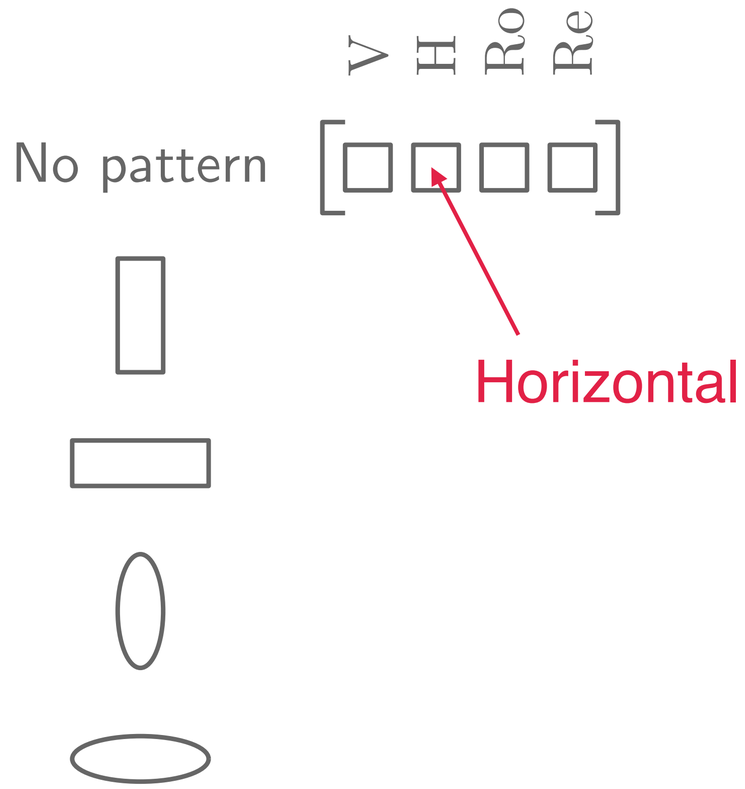

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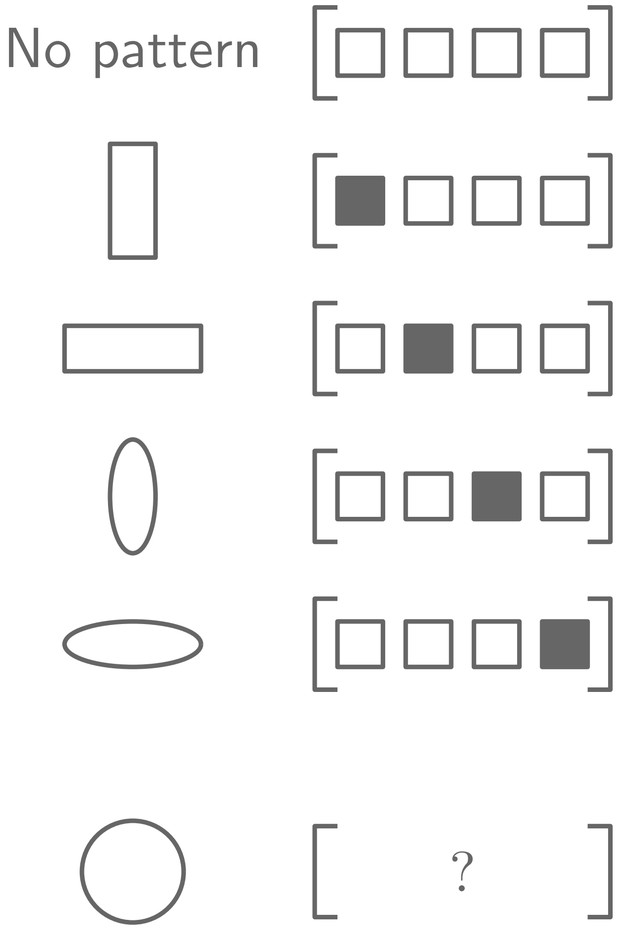

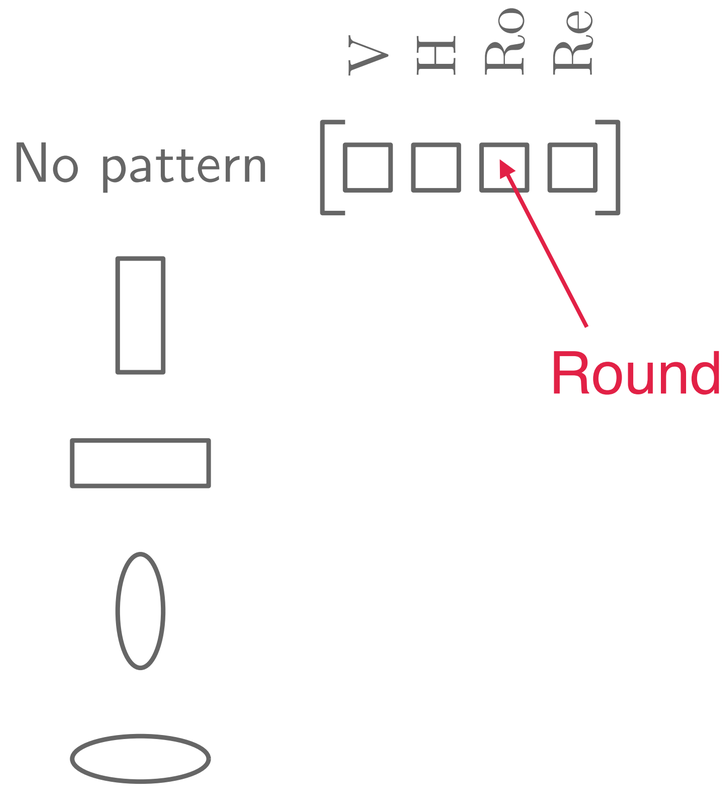

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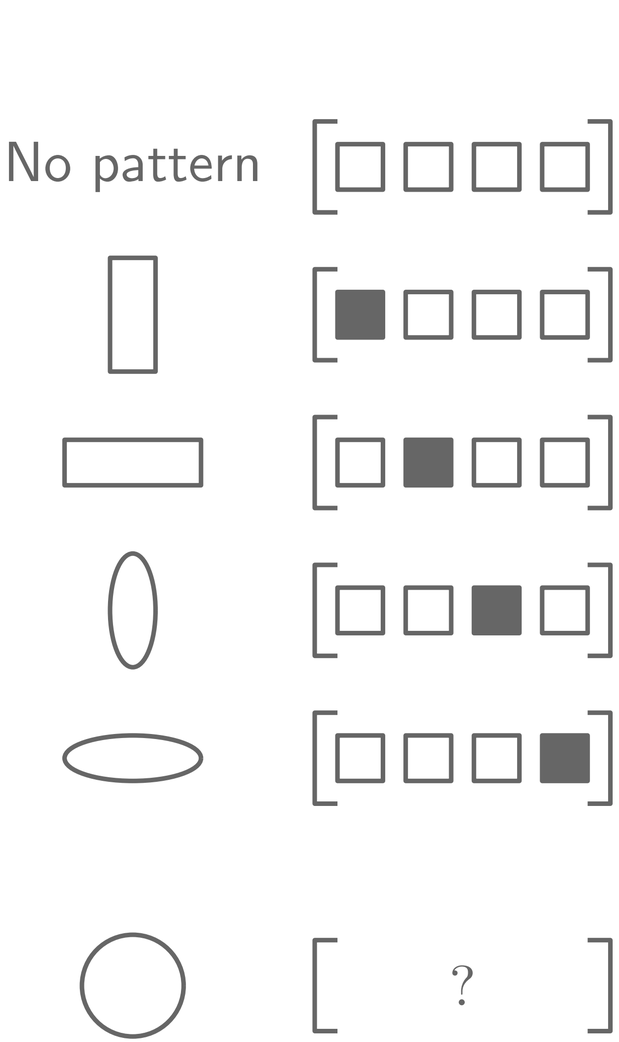

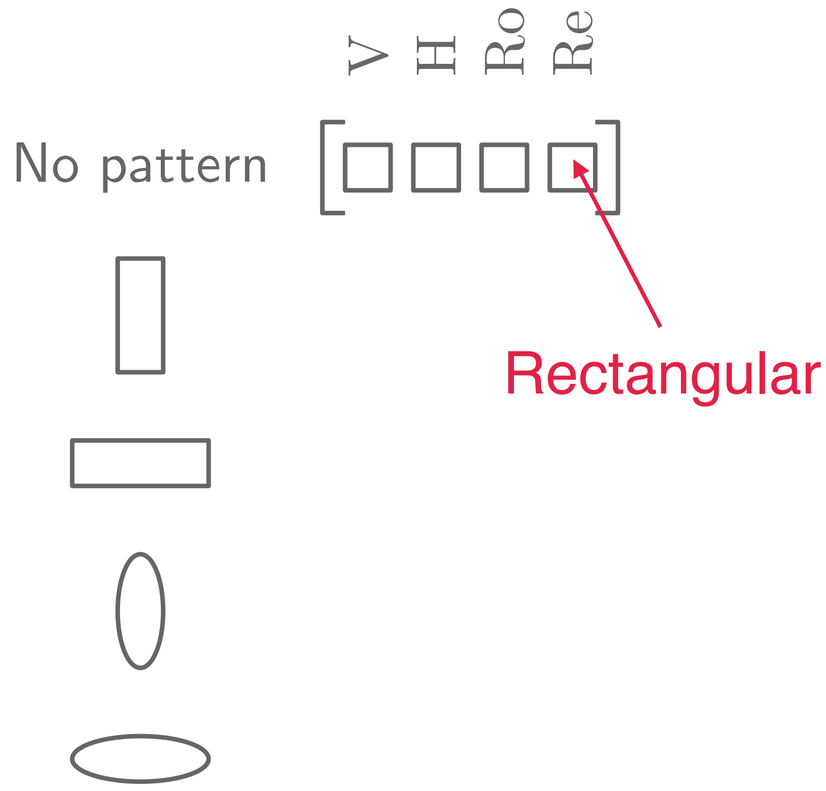

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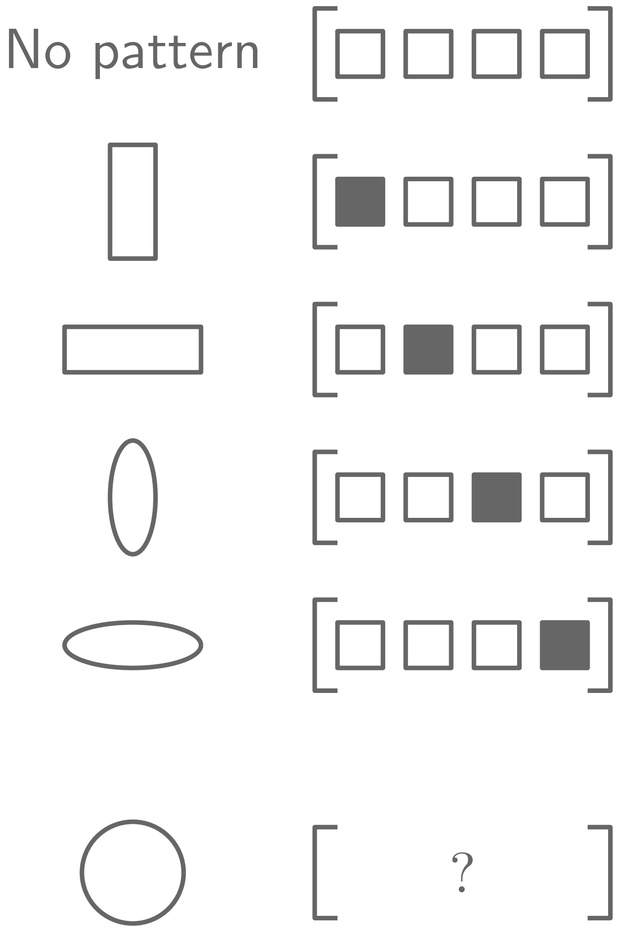

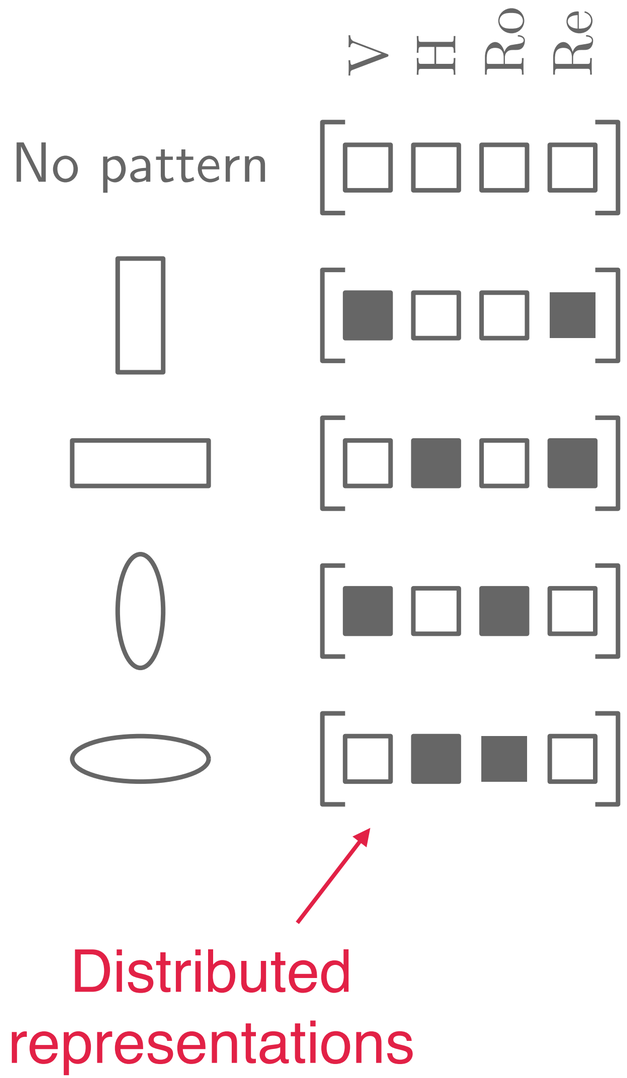

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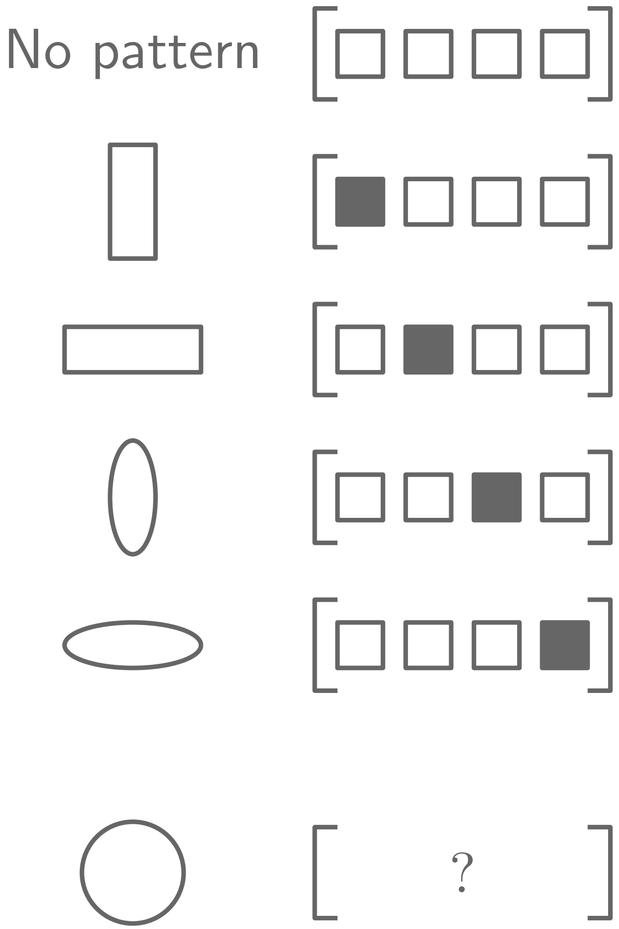

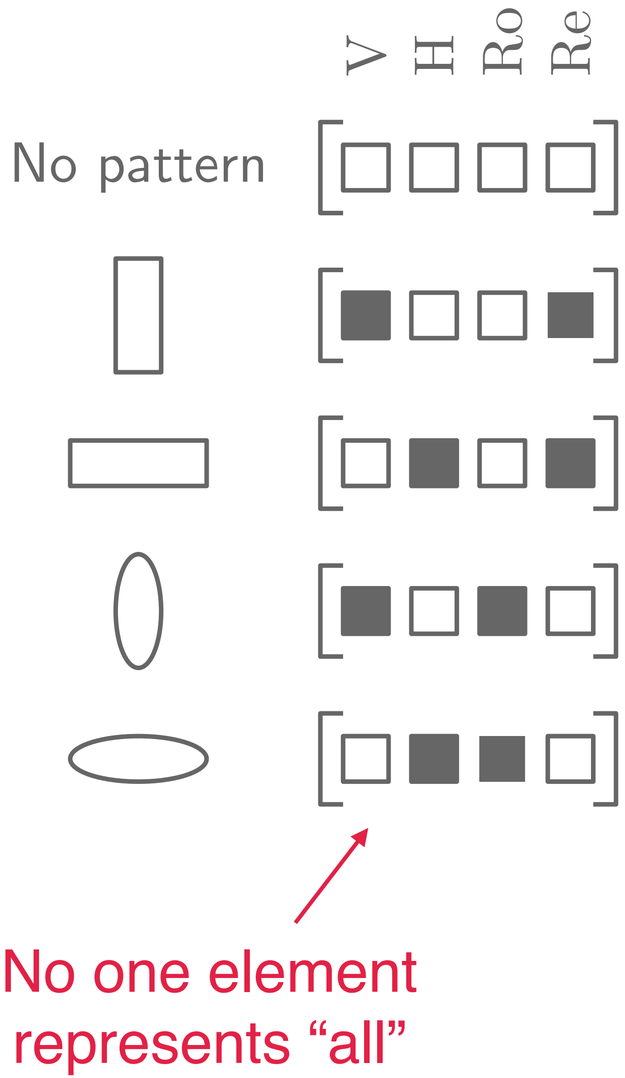

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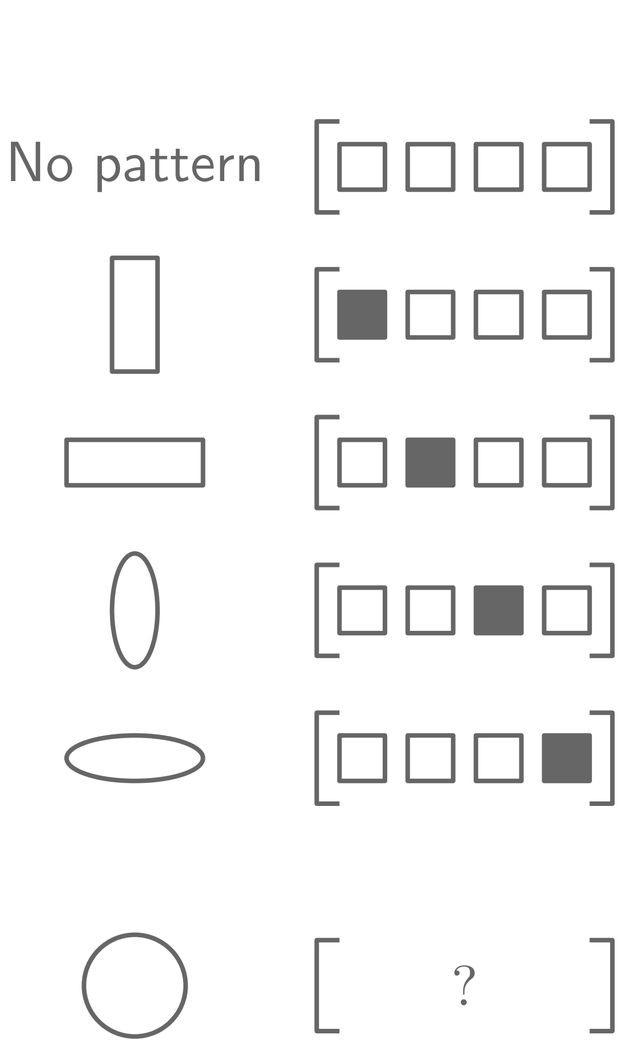
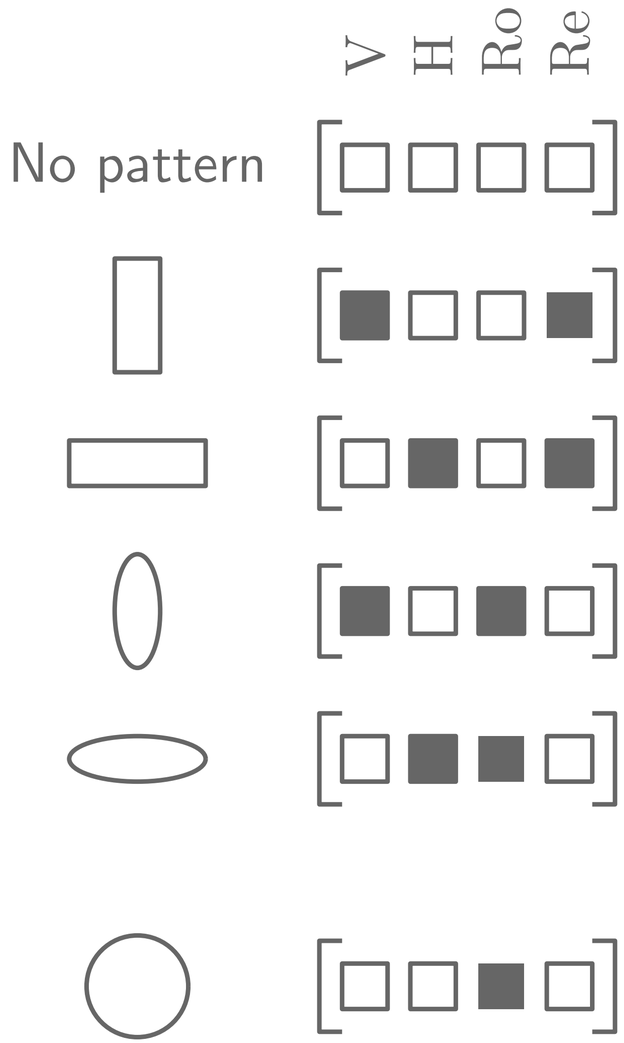




The power of distributed representations

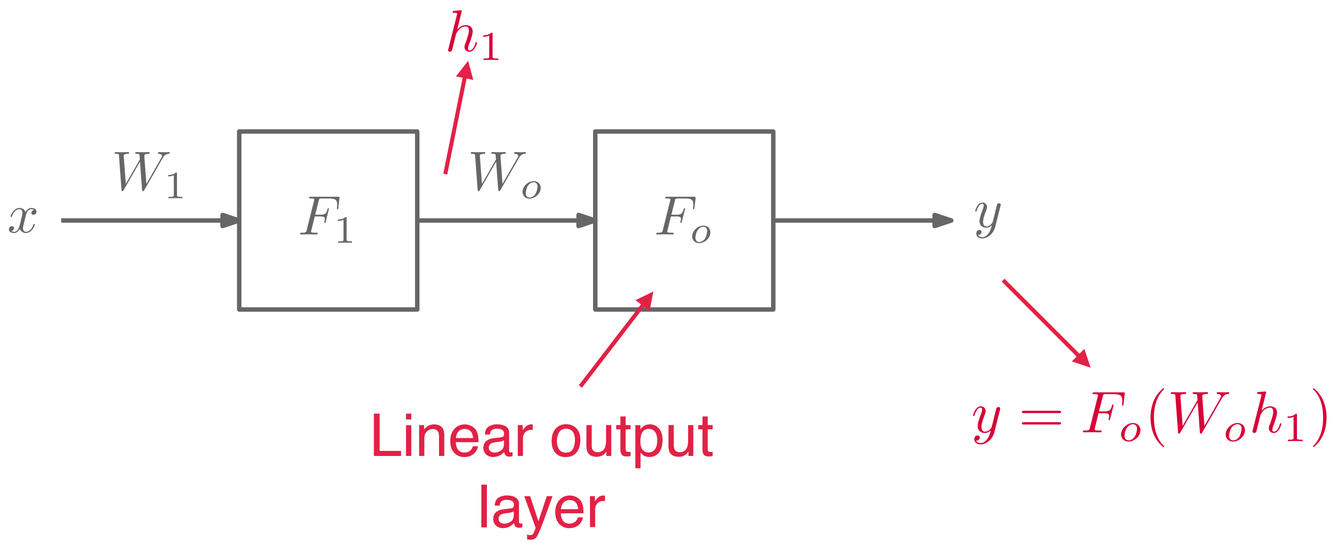
- Distributed representations are:
  - More compact (a vector with N attributes may be used to represent up to $O(2^N)$ objects)
  - More powerful (may generalize in a meaningful way)

Learning representations

- What is a good representation?
  - Retains all the relevant information
  - Compact

- Can we have a neural network learn to do that?

Learning representations



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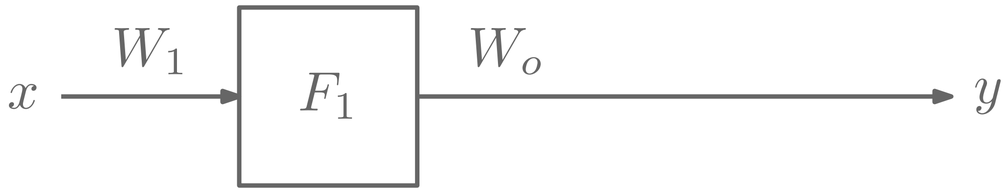

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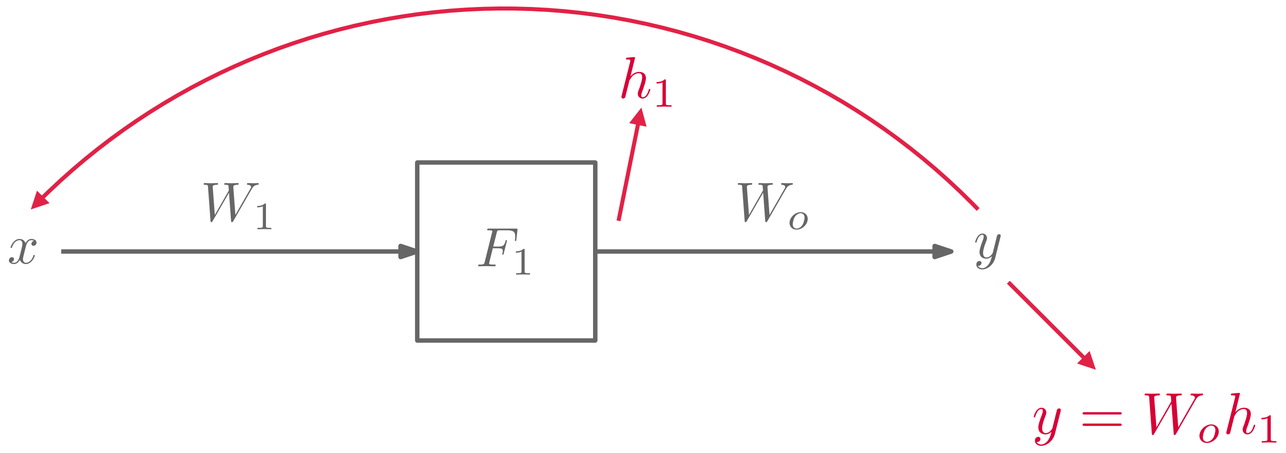
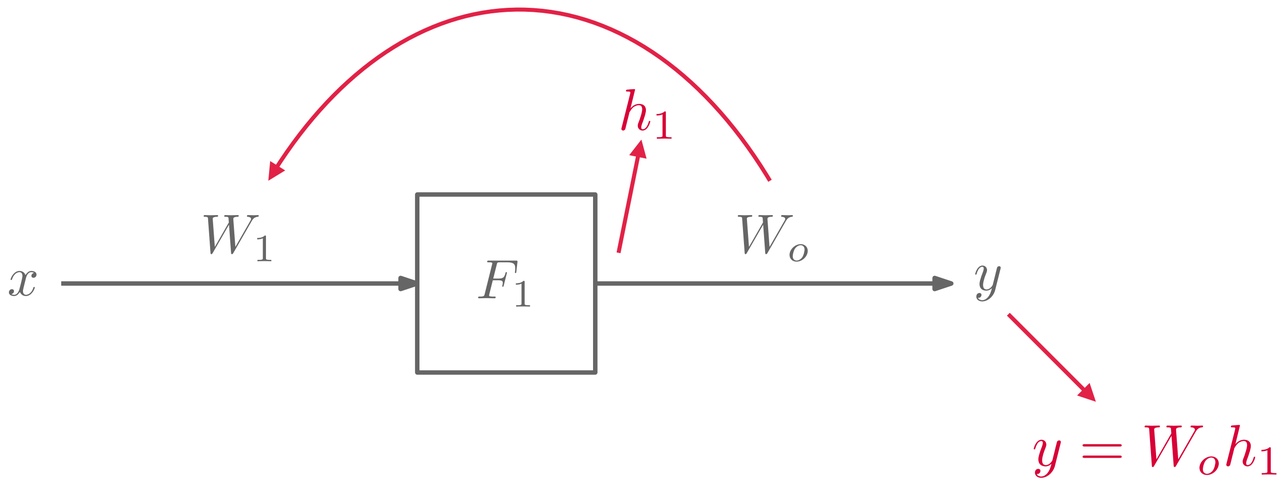


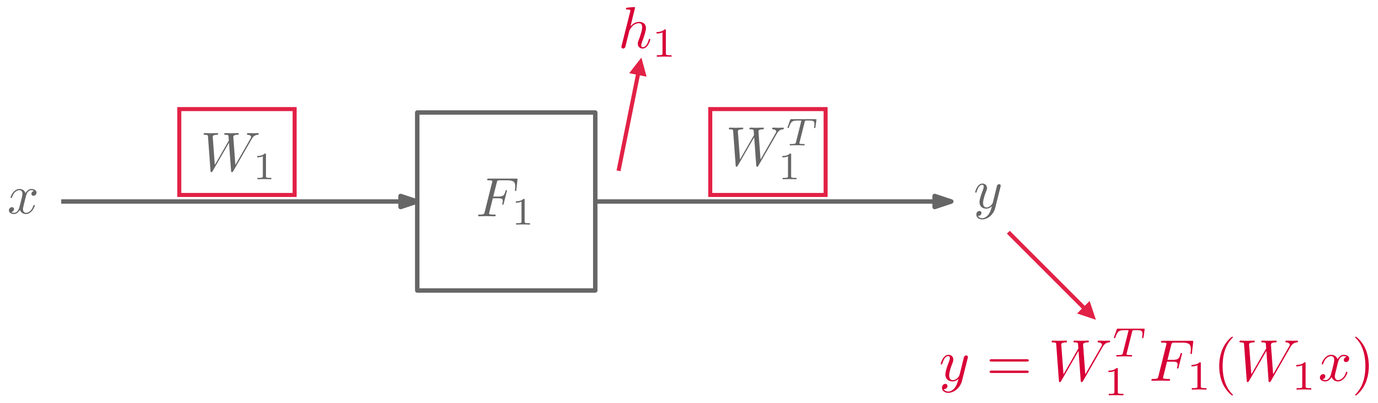
1. Capturing all relevant information → We should be able to reconstruct the input *x* → Goal: Minimize distance between *y* and *x*, $\|y - x\|^2$

Learning representations



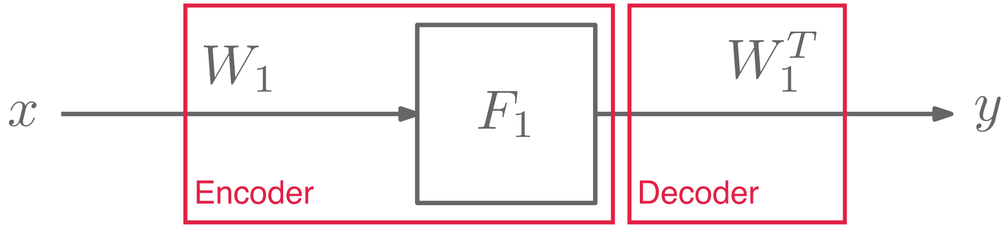
1. Capturing all relevant information → We should be able to reconstruct the input *x* → Force W_o and W_1 to be similar

Learning representations



2. Compact ⟶ We make dim(h_1) < dim(x) ⟶ W_1 is $m \times n$ with $m < n$

Auto-encoder



- We train the neural network so that it reconstructs the input in the output
- Encoder computes a compact representation:

$$h_1 = F_1(W_1 x)$$

Code

- Decoder reconstructs input from learned representation:

$$y = W_1^T h_1$$

Interesting facts

- If F_1 is linear and we use the squared loss, the optimal auto-encoder is the same as PCA
- Auto-encoders were historically used for unsupervised pre-training of deep NNs:
  - (Pre-)Train one layer at a time as an auto-encoder
  - Once all hidden layers are pre-trained, add output layer and train everything as usual

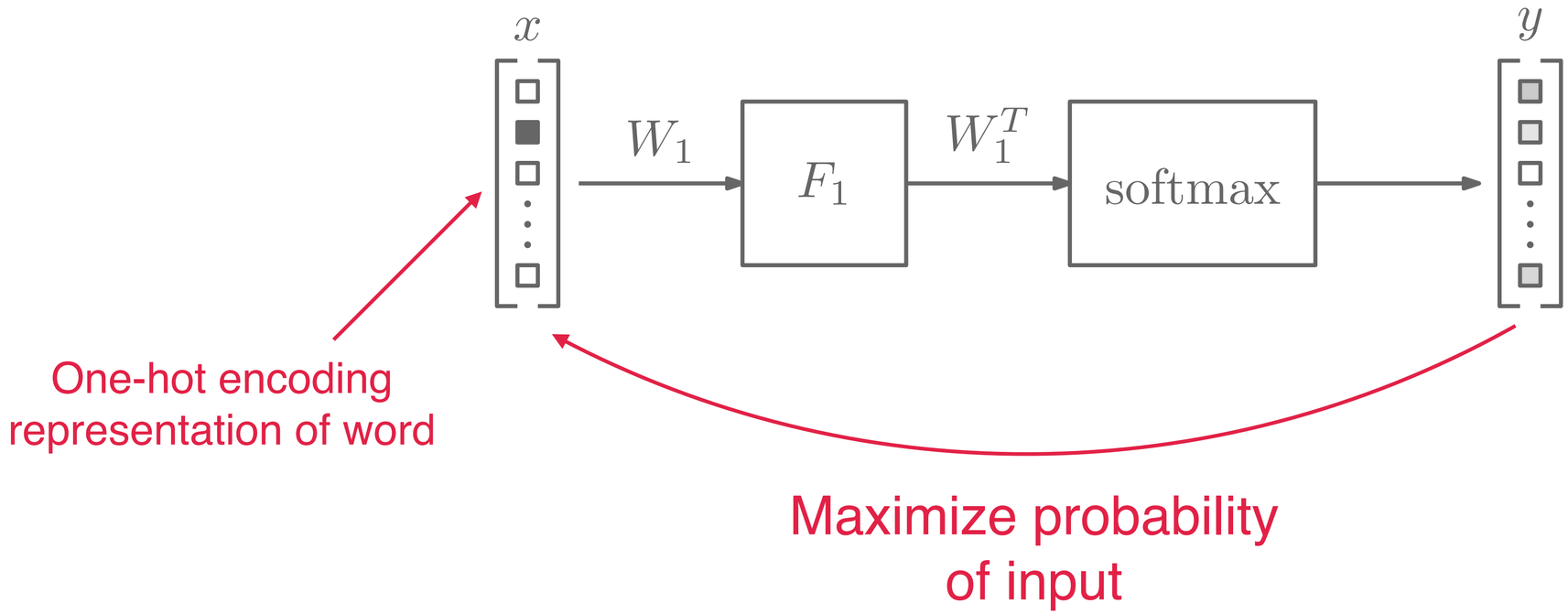
Variations of auto-encoders

- Sparse auto-encoders: Add L^1 regularization to encourage sparse representations
- Denoising auto-encoders: Add noise to the input, training the AE to reconstruct denoised input
- Variational auto-encoders: Learn a probabilistic generative model (more on this in the last lecture)

Now, we move to text

Learning representations of text

- How can we apply these ideas to learn good representations of text/words?



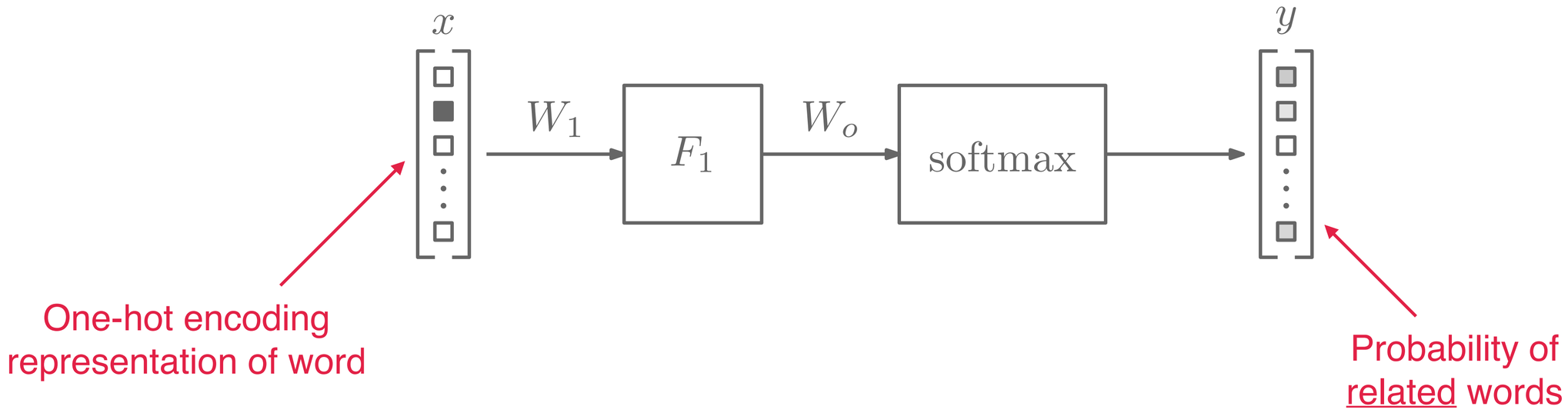
Learning representations of text

- Such naive approach learns “arbitrary” representations for words
- Is it possible that semantically related words have related representations?

Context

Learning representations of text

- Idea: Represent a word in terms of its ability to predict its context



Learning representations of text

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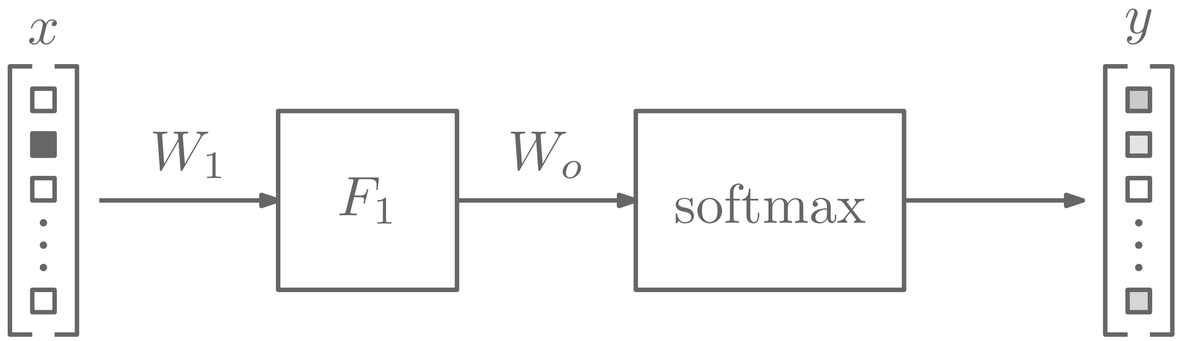

Today we move to text

Learning representations of text

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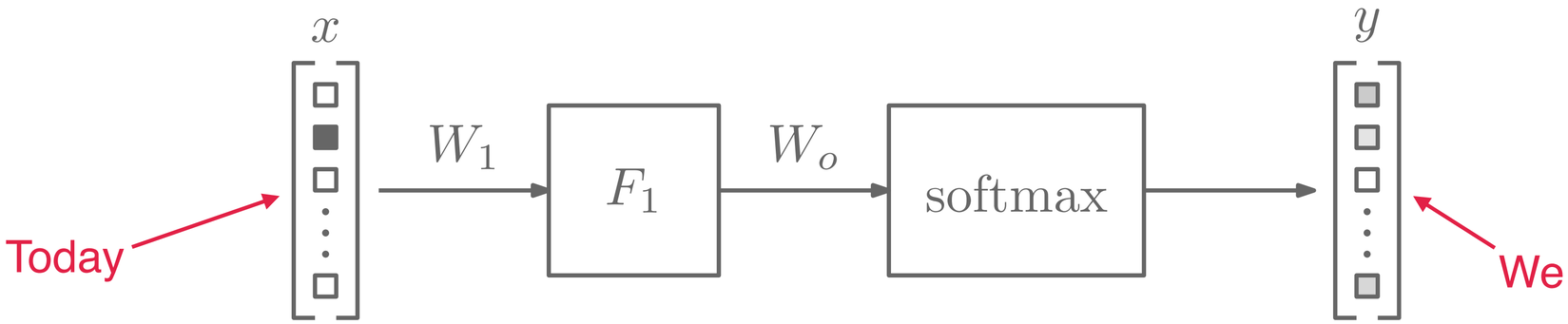

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Learning representations of text

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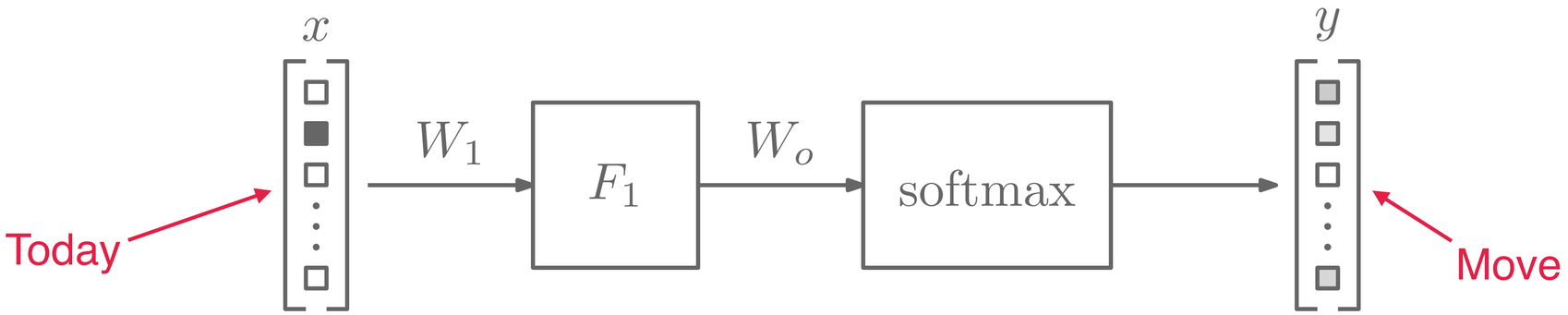

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Learning representations of text

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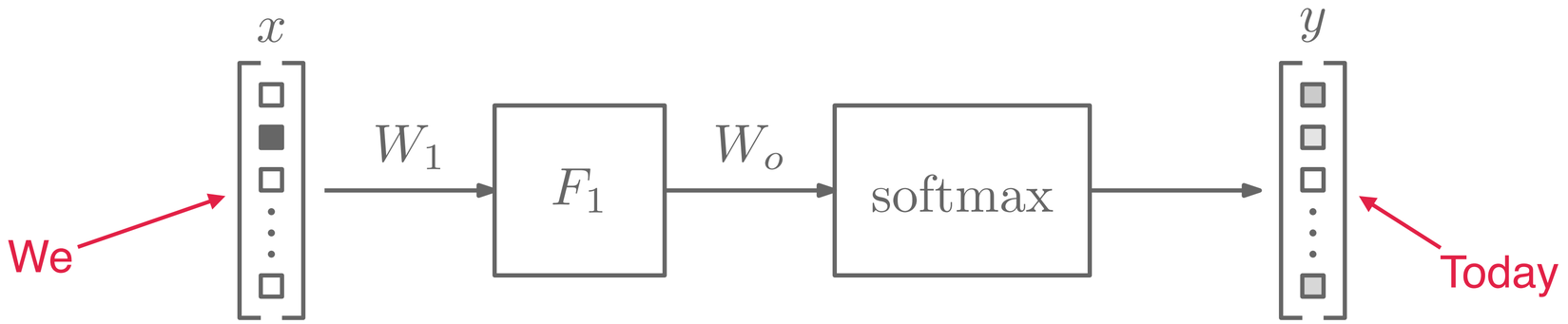

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Learning representations of text

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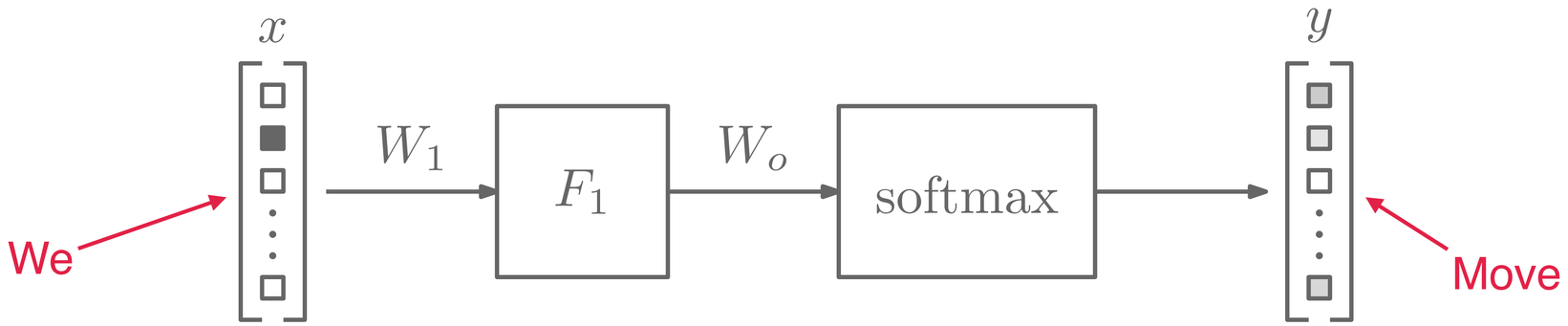

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Learning representations of text

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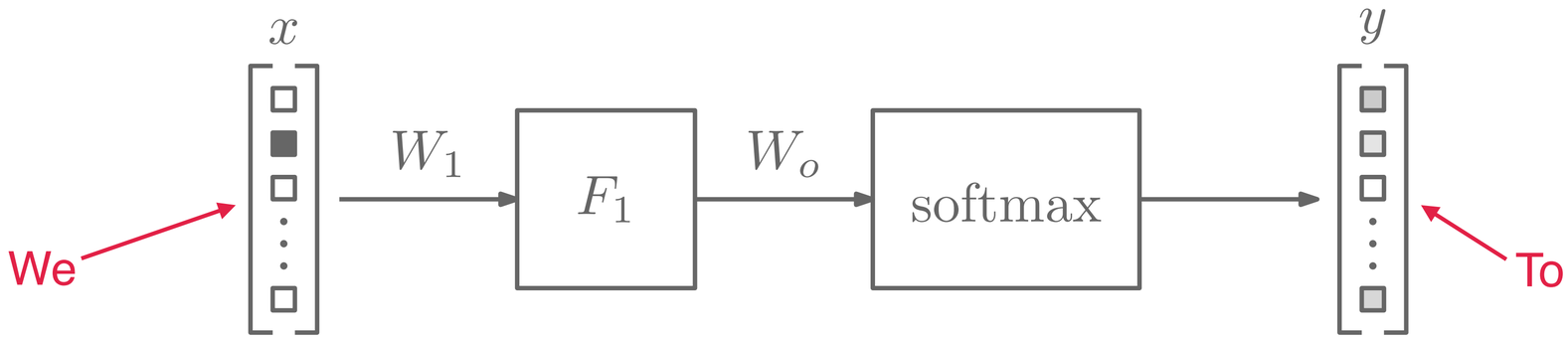
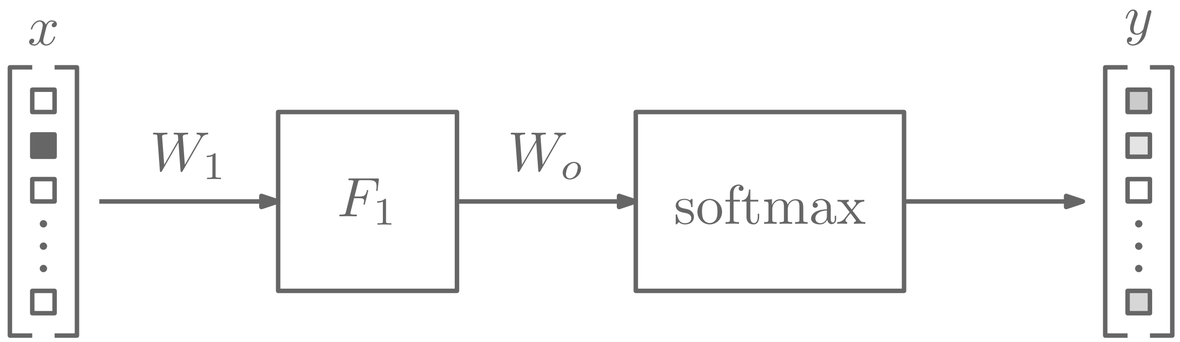


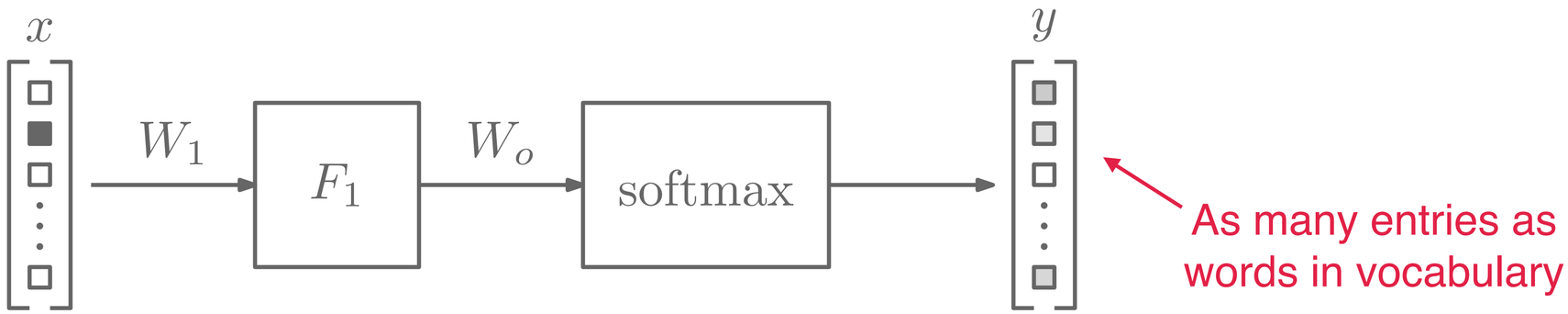
Today	we	move	to	text

Word2vec



- The previous approach is known as word2vec (skipgram model)
- Typically used with linear F_1
- The resulting representation is known as a word embedding
  - The word embedding of the ith word in the vocabulary corresponds to the ith column of W_1

Negative sampling in word2vec



- A difficulty in the implementation of the word2vec model above is the size of the softmax for large vocabularies
- If model is trained with softmax output, training will be very slow

Negative sampling in word2vec

- Output of the word2vec network:

$$[y]_c = \frac{\exp(s_\theta(c, w))}{\sum_{c'} \exp(s_\theta(c', w))} \approx p(c \mid w)$$

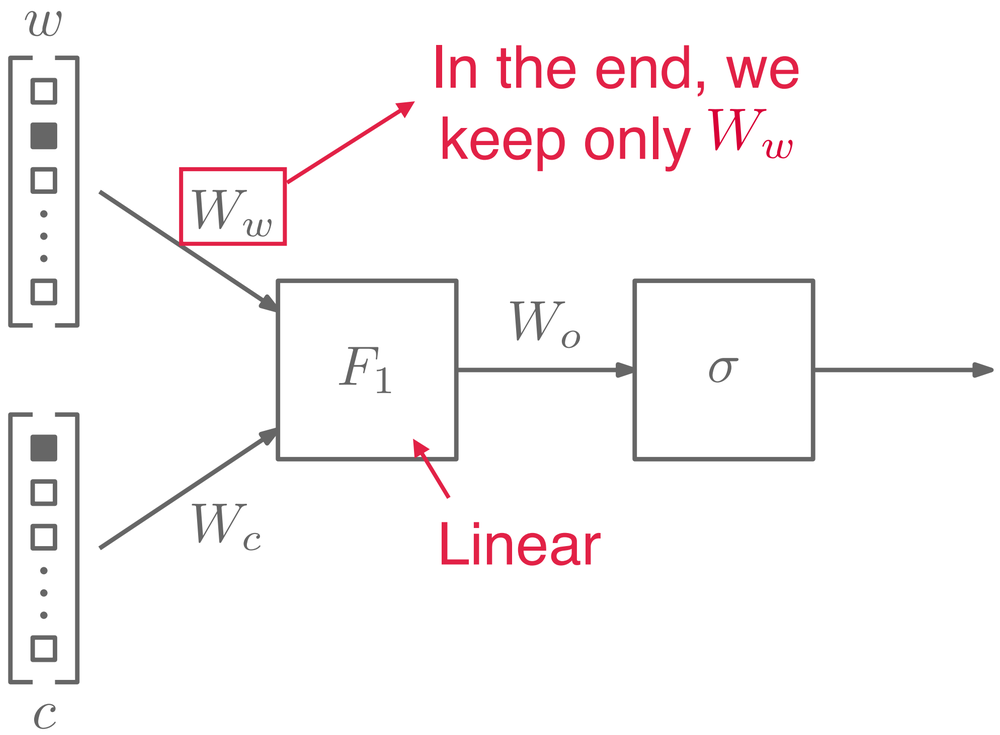
Summation over all vocabulary

Our target distribution

Negative sampling in word2vec

- Suppose that:
  - We sample a pair (*c*, *w*) from the dataset
  - We build pairs (*c*', *w*), where *c*' is selected randomly from the vocabulary
- We train a binary classifier to distinguish “true pairs” from “false pairs”

Negative sampling in word2vec



In the end, we keep only W_w

Linear

$$y \approx \mathbb{P}[\text{pair is true} \mid (c, w)]$$

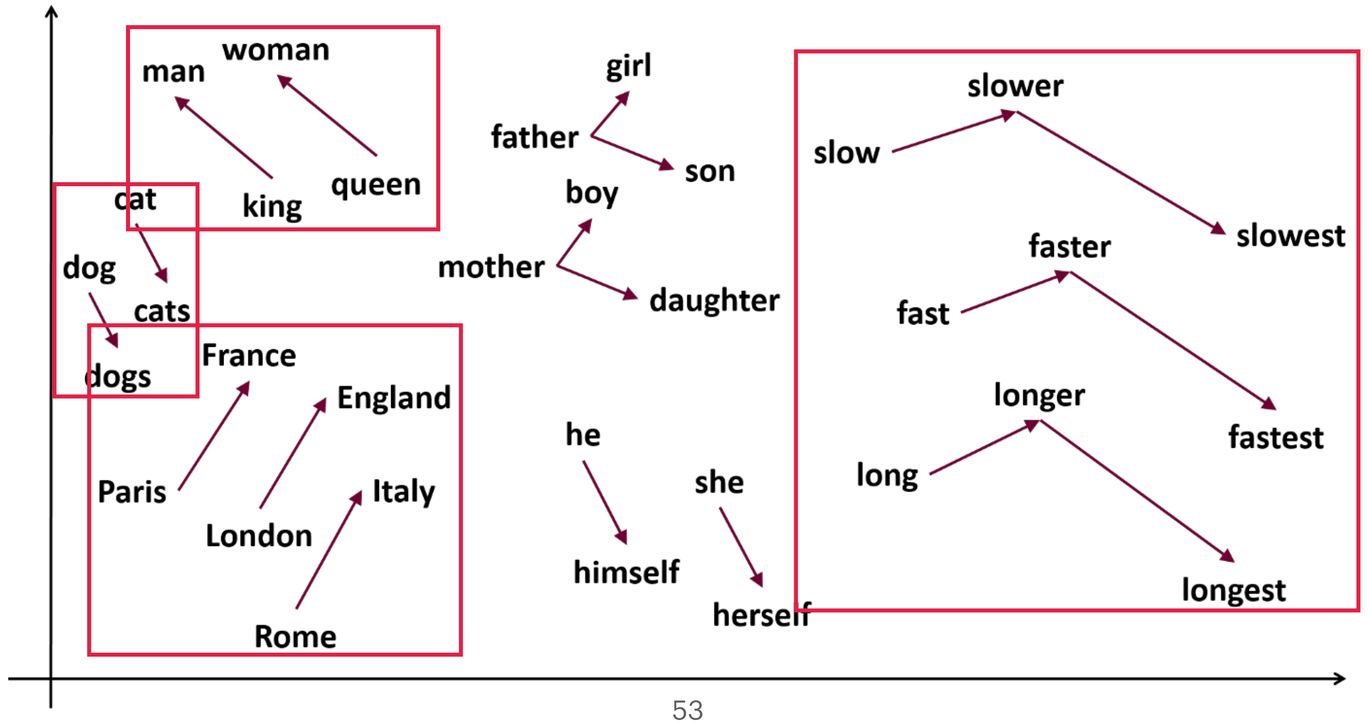
Approximately

$$\frac{1}{1 + \exp(-s_\theta(w, c))}$$

Same quantity as before

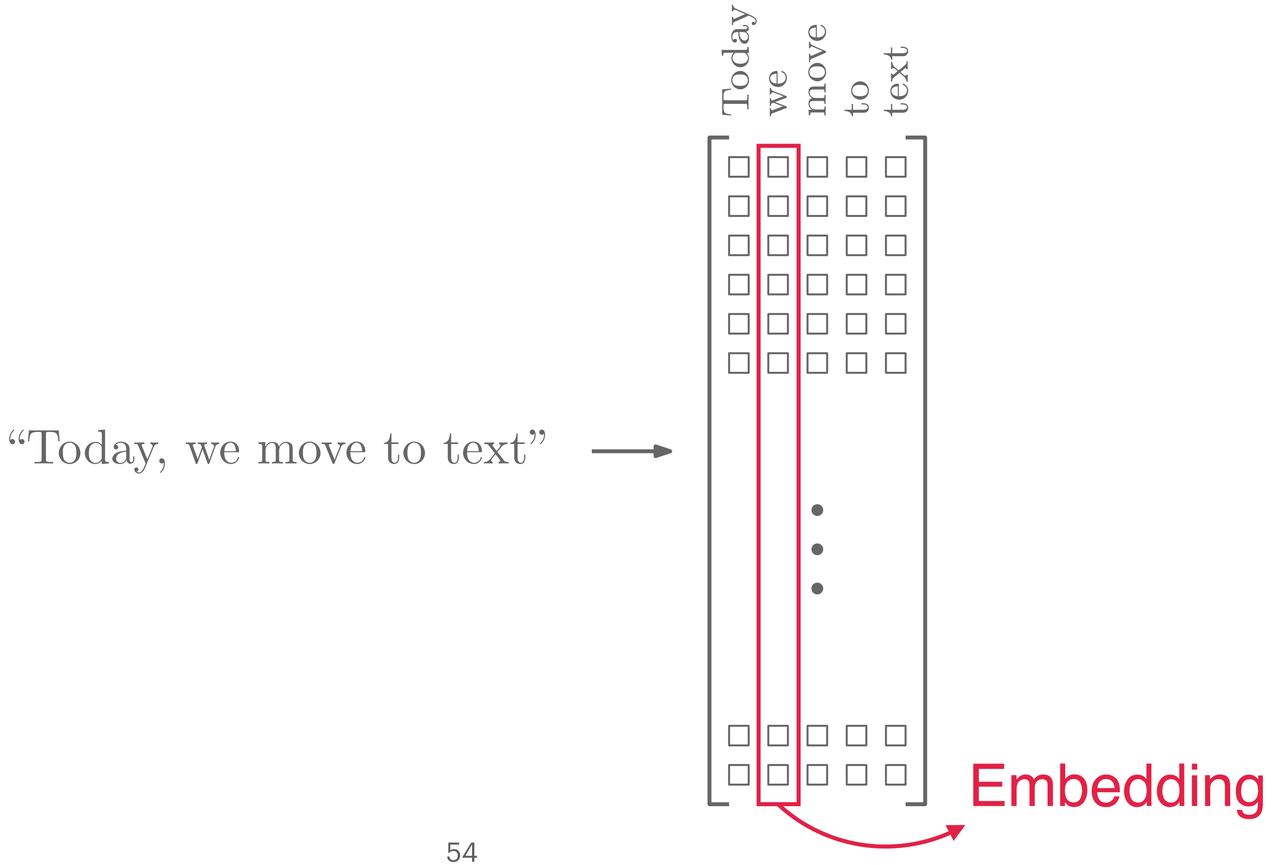
Word2vec

- We can visualize the representations learned by word2vec by projecting them into a low-dimensional (2D) space:



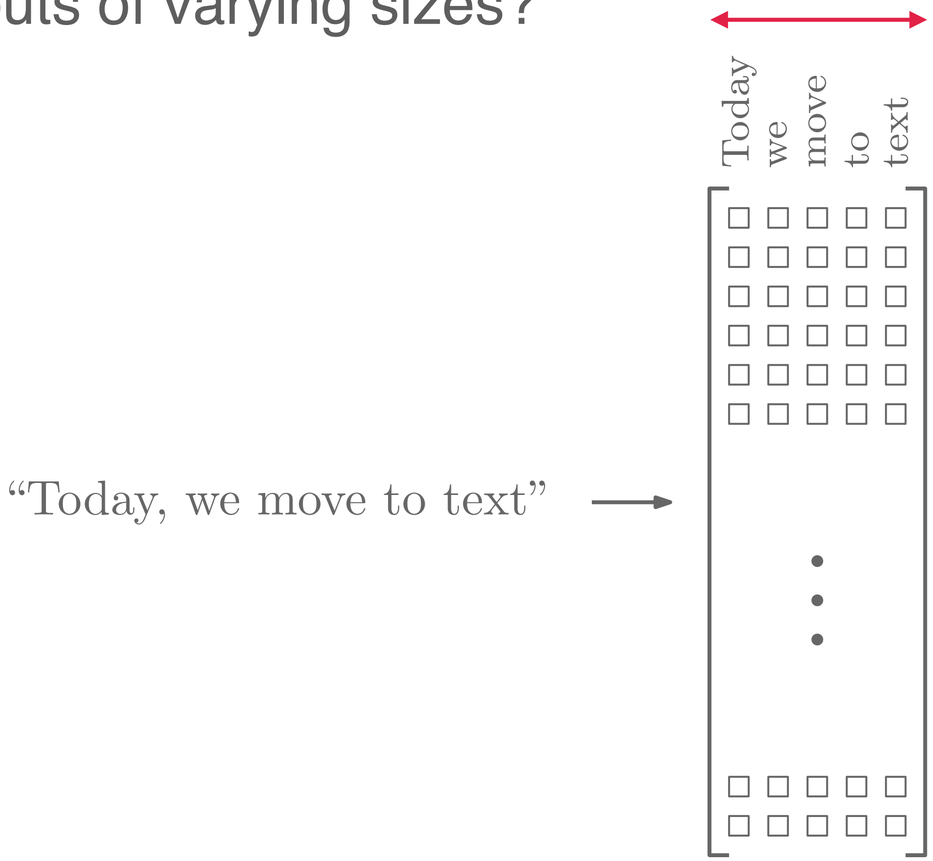
Problem n. 1

- How do we represent text as a vector/matrix of numbers?



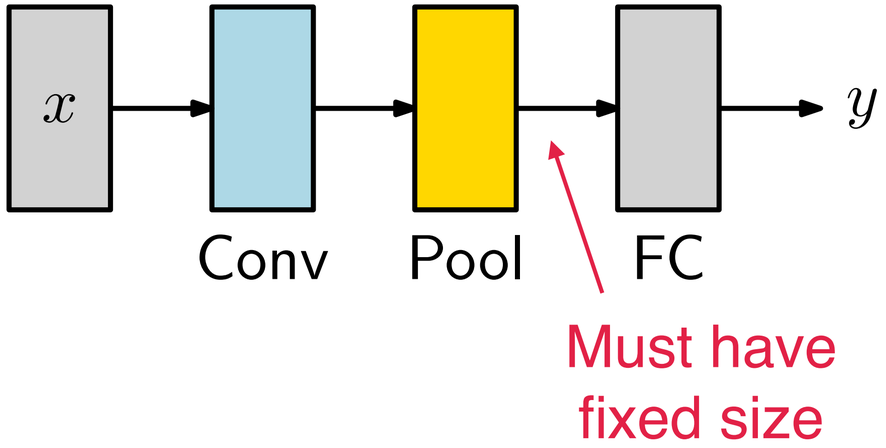
Problem n. 2

- How do we deal with inputs of varying sizes?

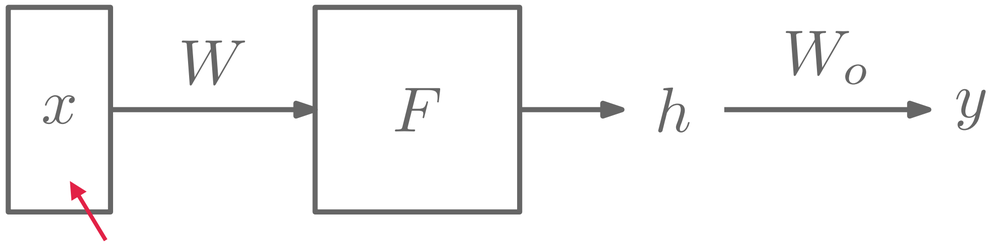


Recurrent neural networks

Convolutional neural networks

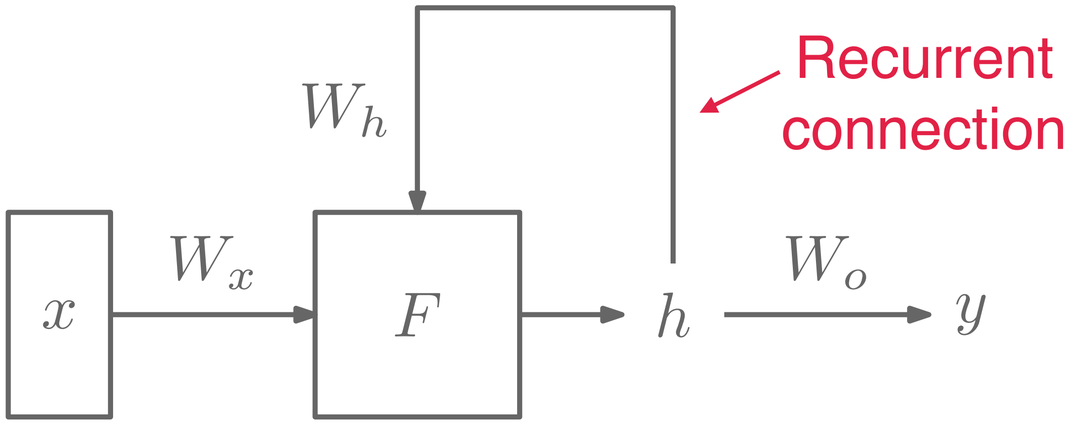


Feed-forward neural networks



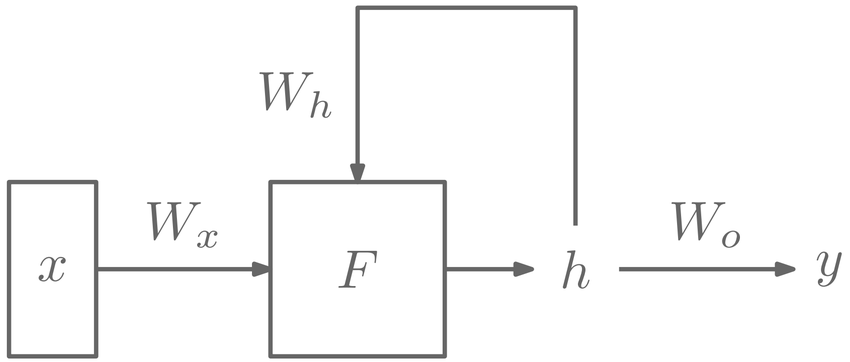
$$h = F(Wx)$$
$$y = W_o h$$

Recurrent neural networks



$$h = F(W_x x + W_h h)$$
$$y = W_o h$$

Recurrent neural networks



- The hidden state *h* stores information from previous inputs
- This means that inputs of varying length (e.g., sentences) are treated as sequences
- The neural network processes one element of the sequence at a time

Unrolling time in RNNs

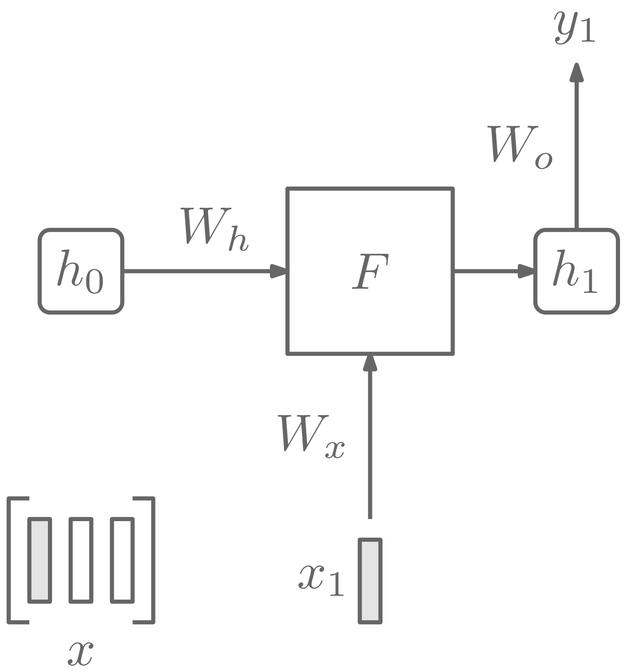
Initial hidden state

Input sequence

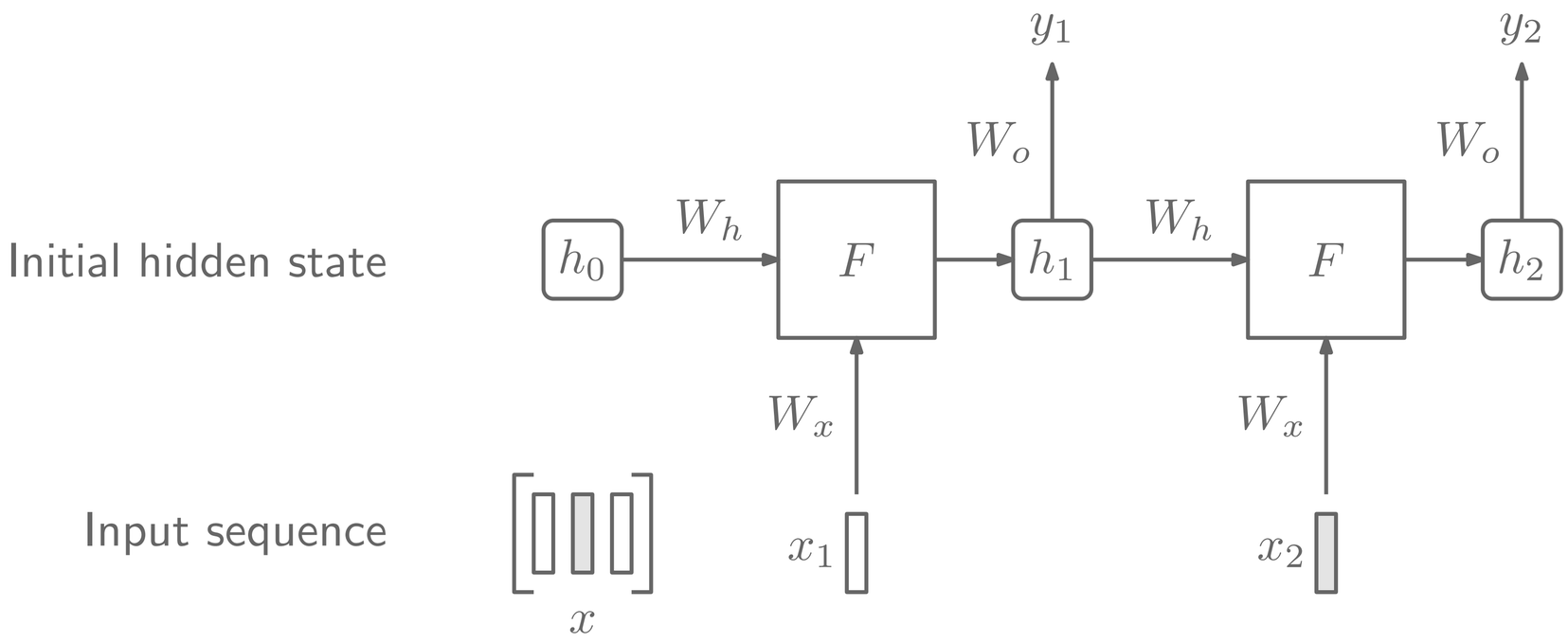
Unrolling time in RNNs

Initial hidden state

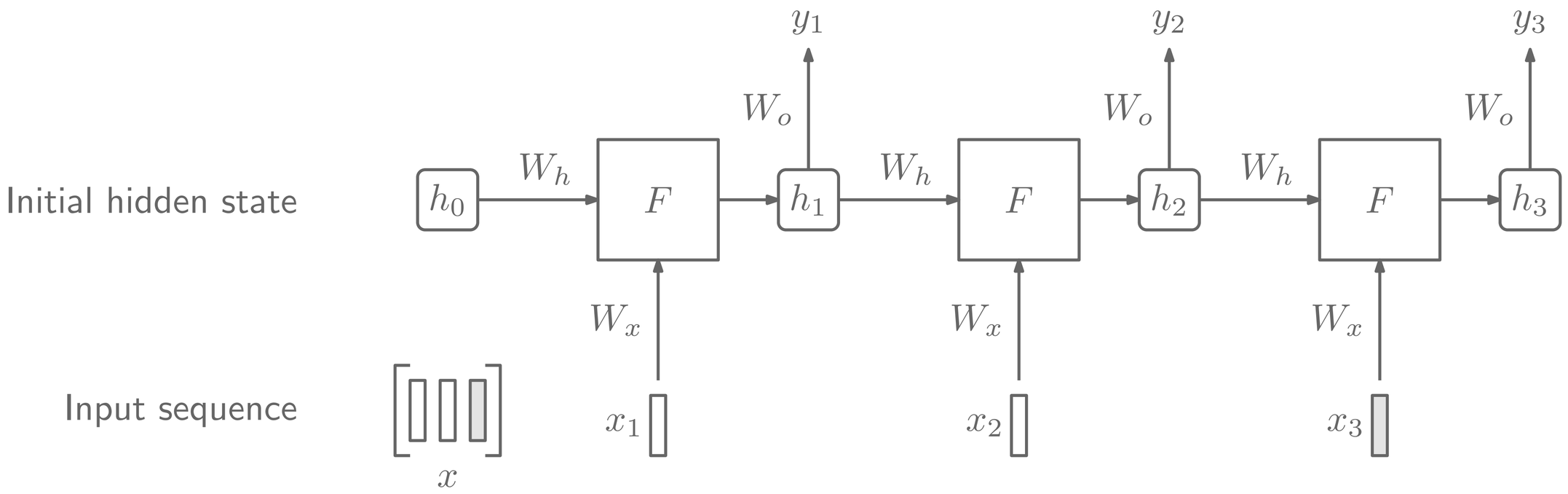
Input sequence



Unrolling time in RNNs

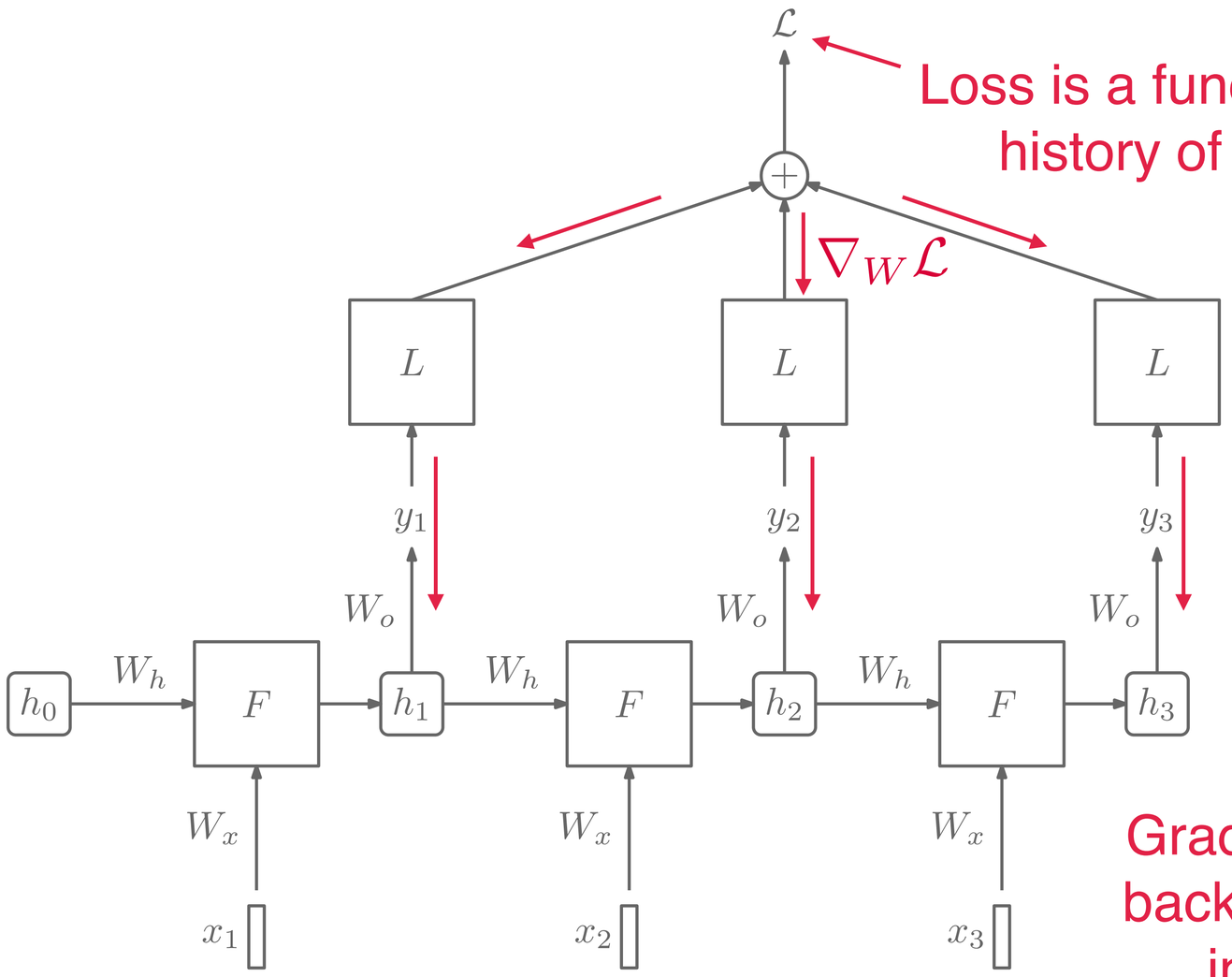


Unrolling time in RNNs



Unrolled graph as a variable network architecture

Unrolling time in RNNs

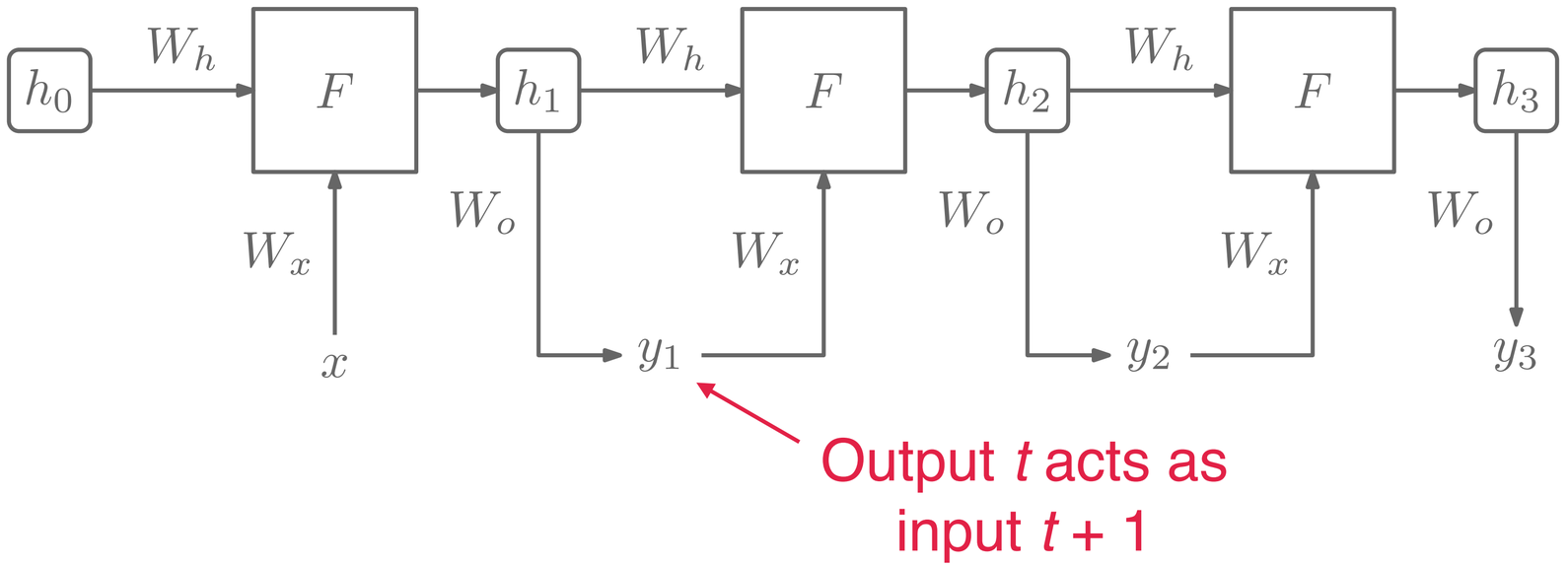


Backpropagation through time

- The unrolled graph is a well-formed computational graph
  - Autograd software can propagate the gradients back as in a standard graph
  - Parameters are shared across time
  - Derivatives aggregated across time
- The process is known as back-propagation through time

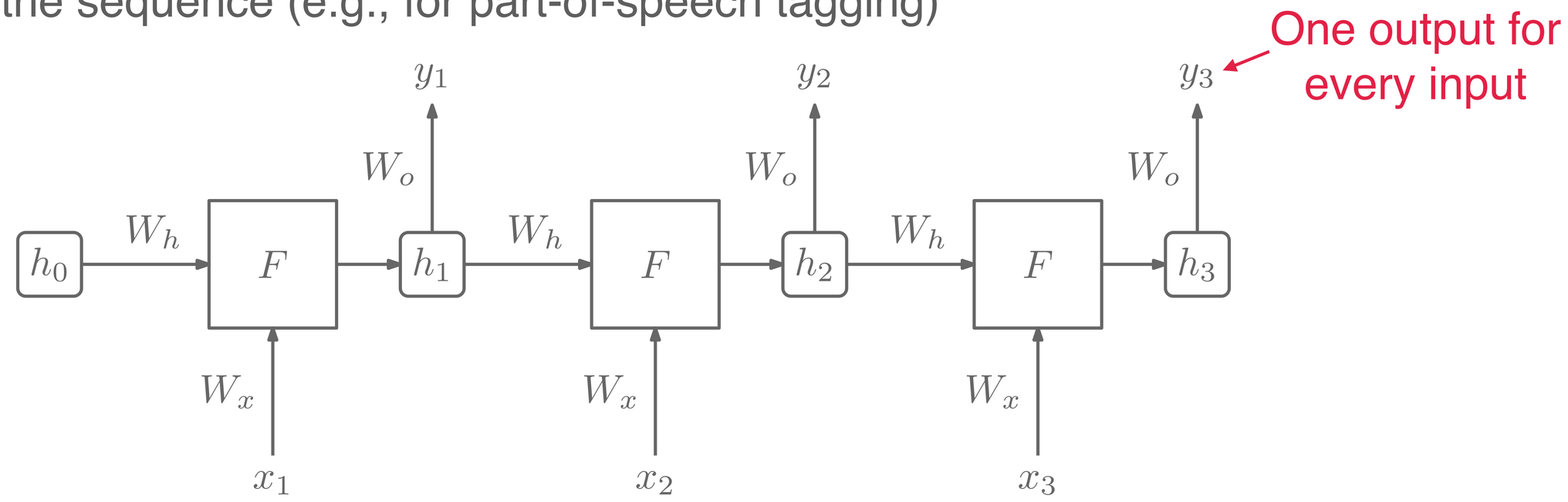
Applications of RNNs

- **Sequence generation:** Network generates a sequence of symbols as an auto-regressive model (e.g., for language generation)



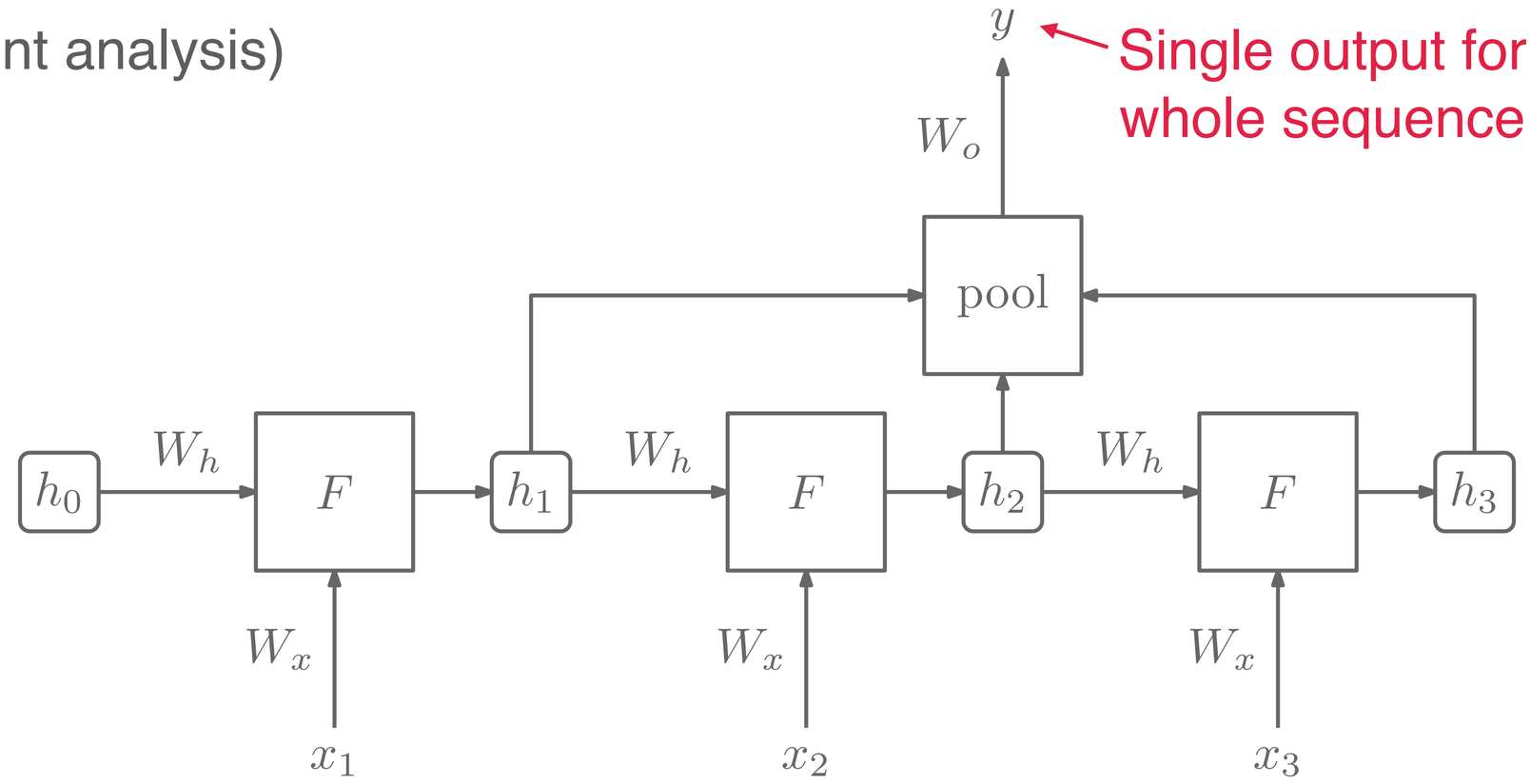
Applications of RNNs

- **Sequence tagging:** Takes a sequence as an input and returns a label/output for each element in the sequence (e.g., for part-of-speech tagging)



Applications of RNNs

- **Pooled classification:** Takes a sequence as an input and returns a single label (e.g., for sentiment analysis)



Sequence generation

Language modeling using RNNs

- Language models are used to represent/describe languages
- Most powerful models are probabilistic:

$$\mathbb{P}[\langle \mathsf{s} \rangle, x_1, x_2, \ldots, x_N, \langle \mathsf{e} \rangle] = \prod_{n=1}^{N+1} \mathbb{P}[x_n \mid x_0, \ldots, x_{n-1}]$$

Probability of a sentence

Probability of a word given previous words

- However, these distributions are too complex to learn

Sequence generation

Language modeling using RNNs

- **RNNs:**
  - Maintain a state vector h_t that is a function of previous state and current input:

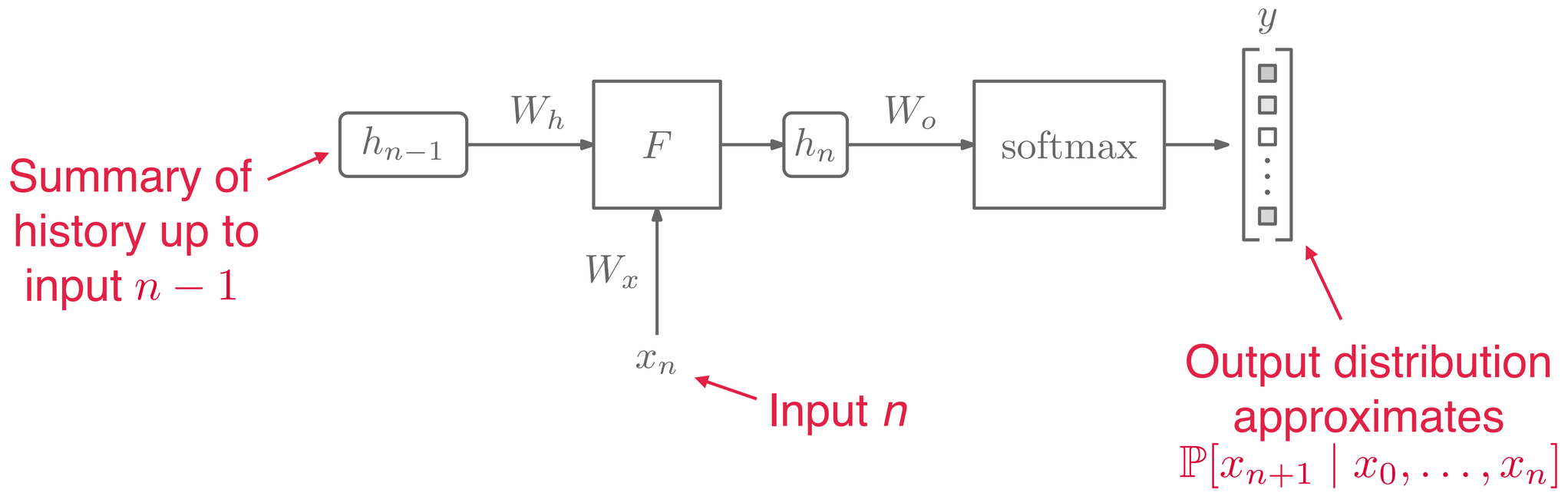
$$h_n = F(W_x x_n + W_h h_{n-1})$$

  - Compute probability of next element:

$$\mathbb{P}[x_{n+1} \mid x_0, \ldots, x_n] = \text{softmax}(W_o h_n)$$

Sequence generation

Language modeling using RNNs

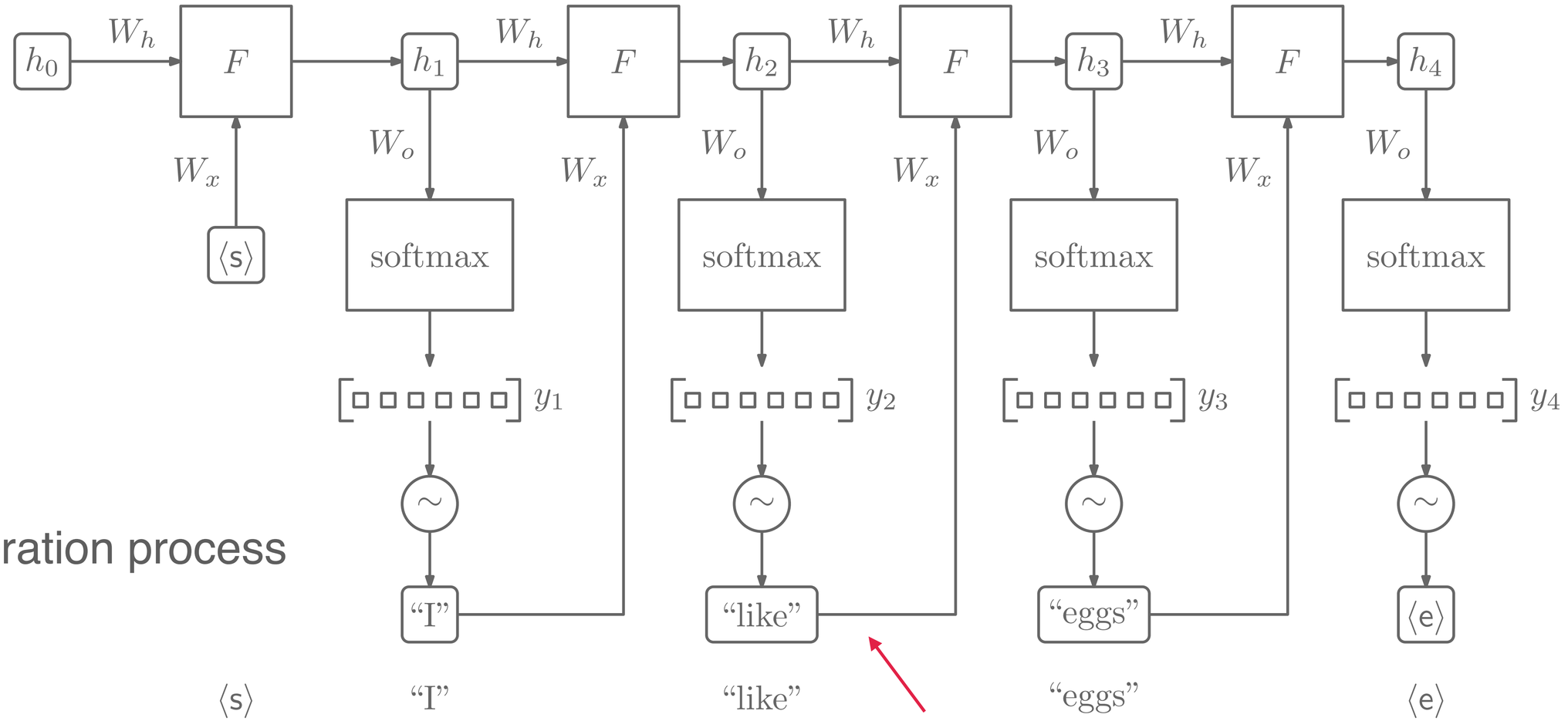


Generation process

- Compute $h_1 = F(W_x x_1 + W_h h_0)$, with $x_1 = \langle s \rangle$
- Sample $x_2 \sim \text{softmax}(W_o h_1)$
- Compute $h_2 = F(W_x x_2 + W_h h_1)$
- Sample $x_3 \sim \text{softmax}(W_o h_2)$
- … etc…

Sequence generation

Language modeling using RNNs



Generation process

Auto-regressive

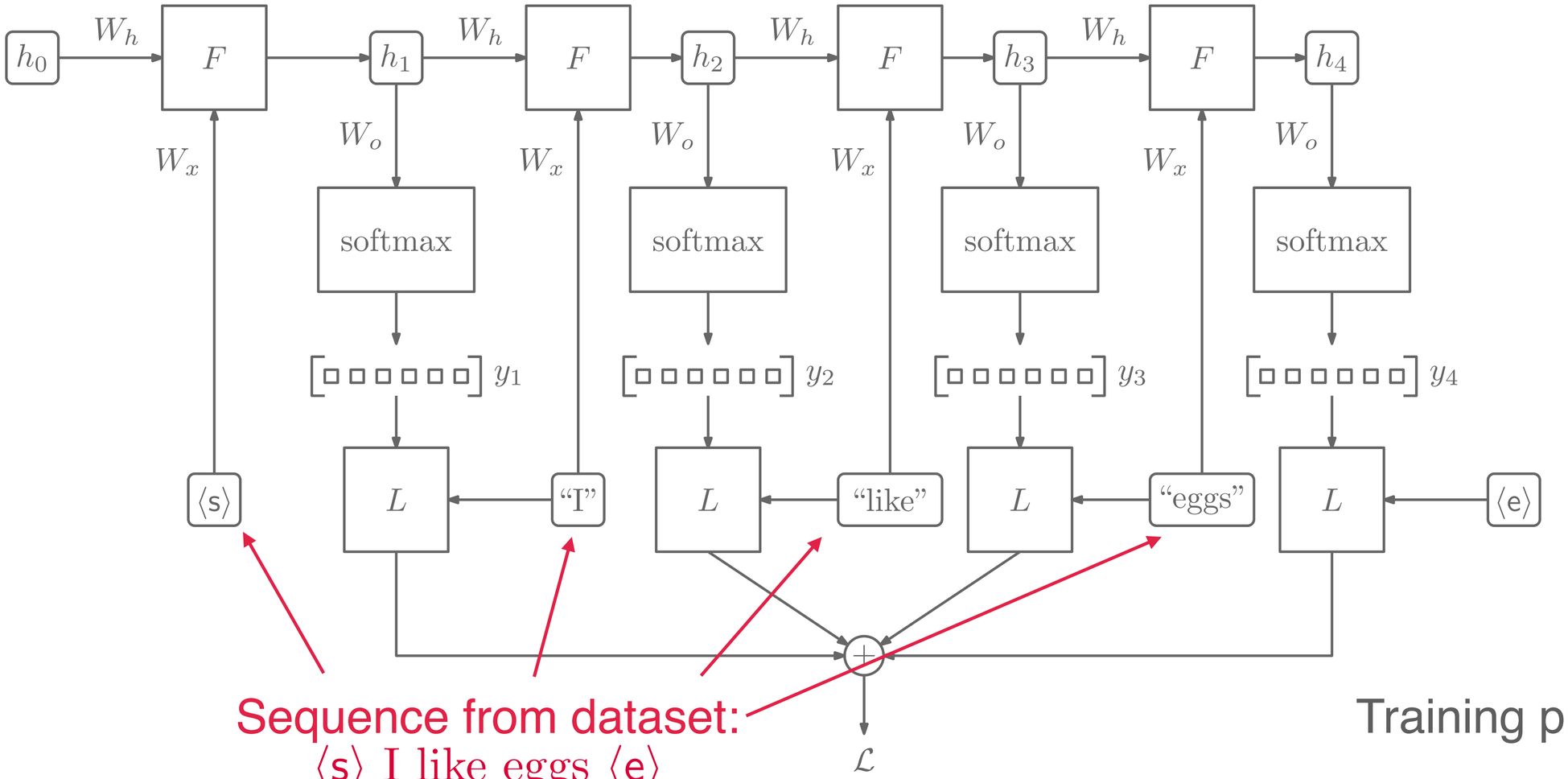
Sequence generation

Language modeling using RNNs

- The network is trained using maximum likelihood estimation
- We optimize the parameters to maximize the likelihood of the sequences/sentences in the dataset
- During training, we feed the network with elements from actual sequences in the dataset (teacher forcing)

Sequence generation

Language modeling using RNNs



Sequence generation

Language modeling using RNNs

- It is also possible to build a character-level language model
  - We will do a simple example in the lab
  - Advantage: Can generate any word, not just words from vocabulary
  - Disadvantage: Needs larger memory…

Sequence tagging

Part-of-speech tagging using RNNs

- Part-of-speech tagging consists of assigning a tag to words in a sentence:

Time	flies	like	an	arrow
noun	verb	prep	det	noun

- There is a high correlation between adjacent words

Sequence tagging

Part-of-speech tagging using RNNs

- **RNNs:**
  - Input is a sequence of word embeddings (x_1, …, x_N)
  - Network maintains a state vector

$$h_n = F(W_x x_n + W_h h_{n-1})$$

  - Compute probability of current element tag:

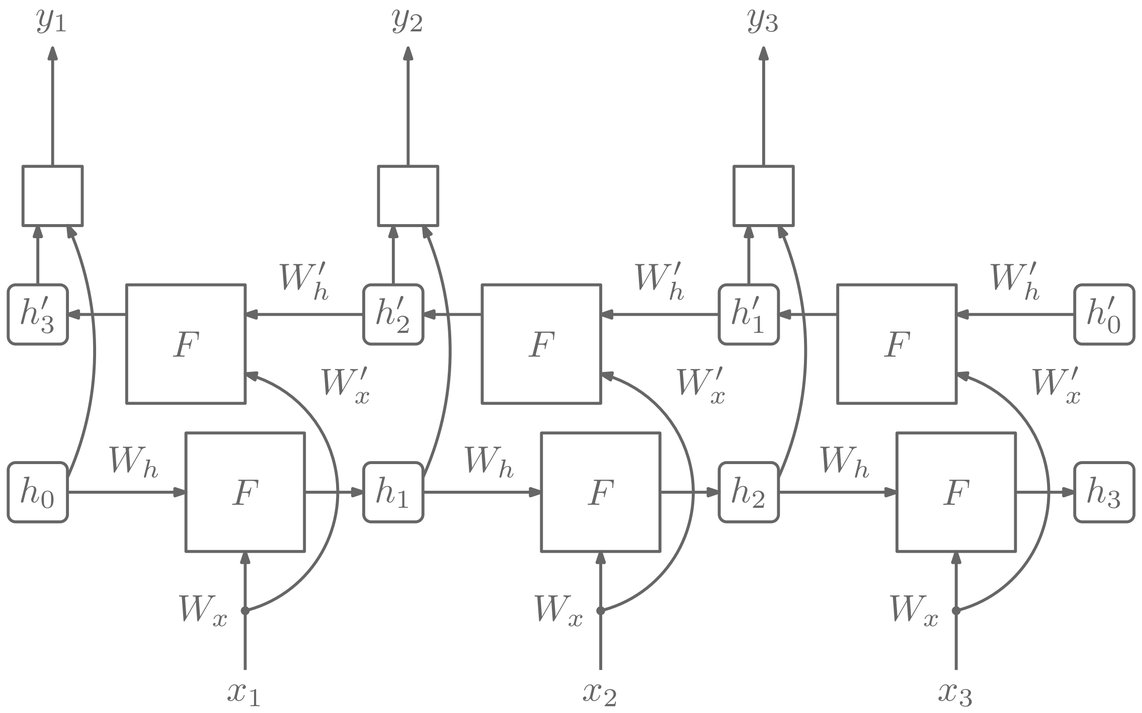
$$\mathbb{P}[c_n \mid x_0, \ldots, x_n] = \mathrm{softmax}(W_o h_n)$$

Tag of element *n*

Sequence tagging

Part-of-speech tagging using RNNs

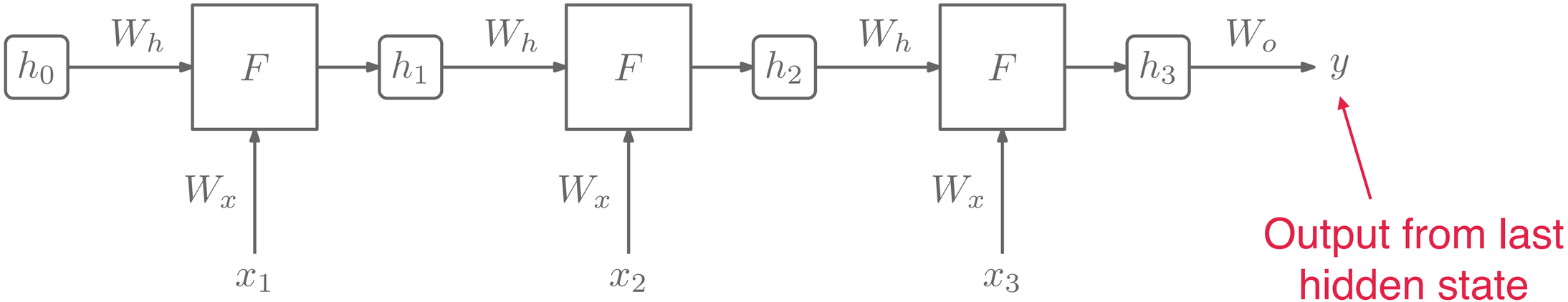
- The model can be improved:
  - The tag is conditioned only on adjacent words to the left
- We can use a bidirectional RNN to condition also on words to the right



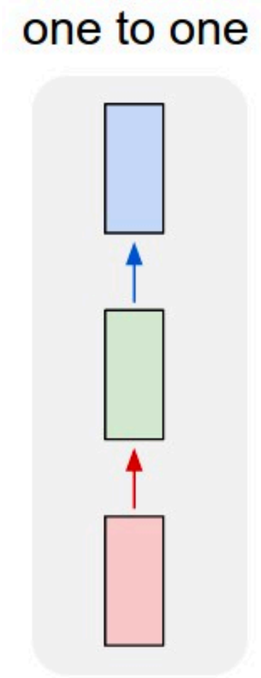
Pooled classification

- What if we want to predict a single label for the whole sequence (e.g., sentiment analysis)?
- We can still use an RNN to capture the information in the input sequence
- We pool the RNN states to a single output
  - Common strategy: use only the last network state

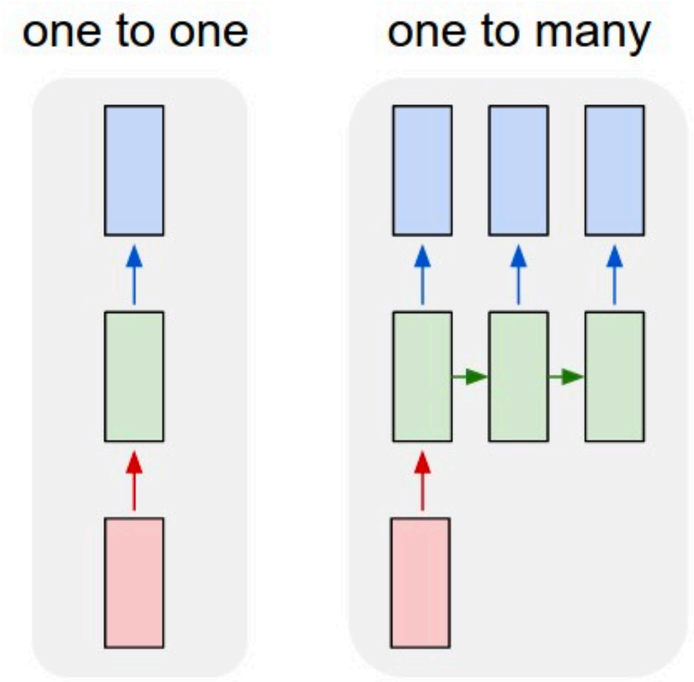
Pooled classification



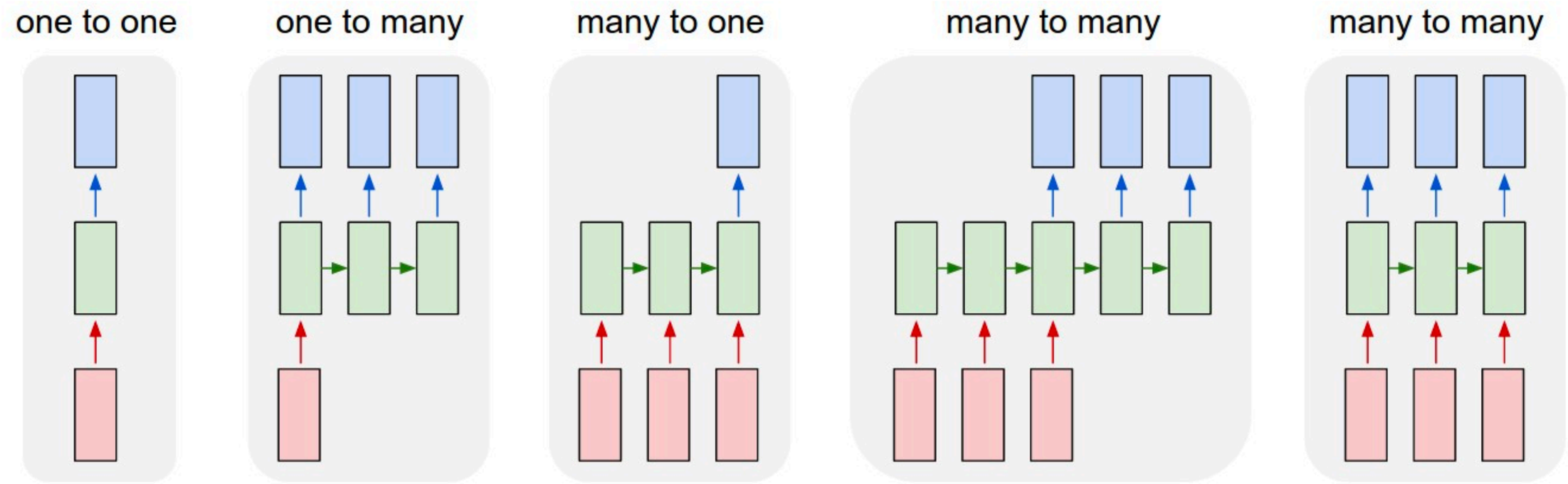
The versatility of RNNs



The versatility of RNNs

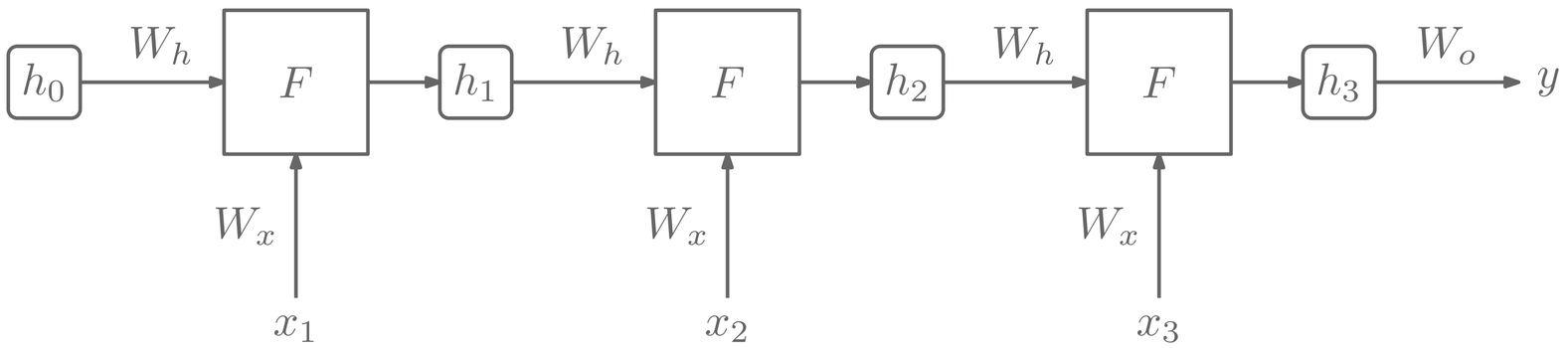


The versatility of RNNs



… however…

Exploding and vanishing gradients

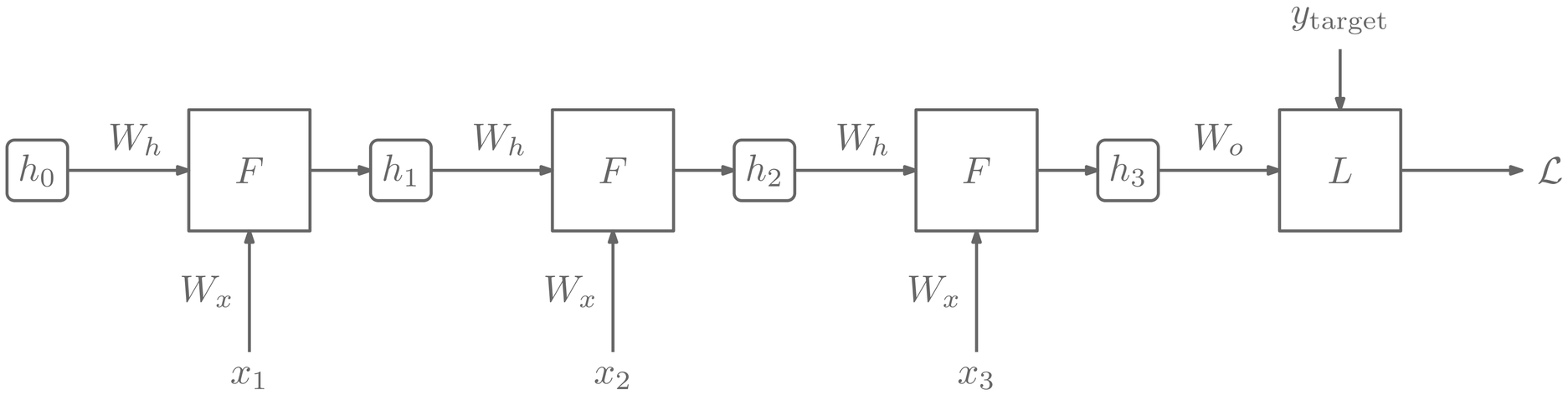


- We have:

$$h_t = F(W_x x_t + W_h h_{t-1})$$
$$y = W_o h_T$$

- What about the gradient?

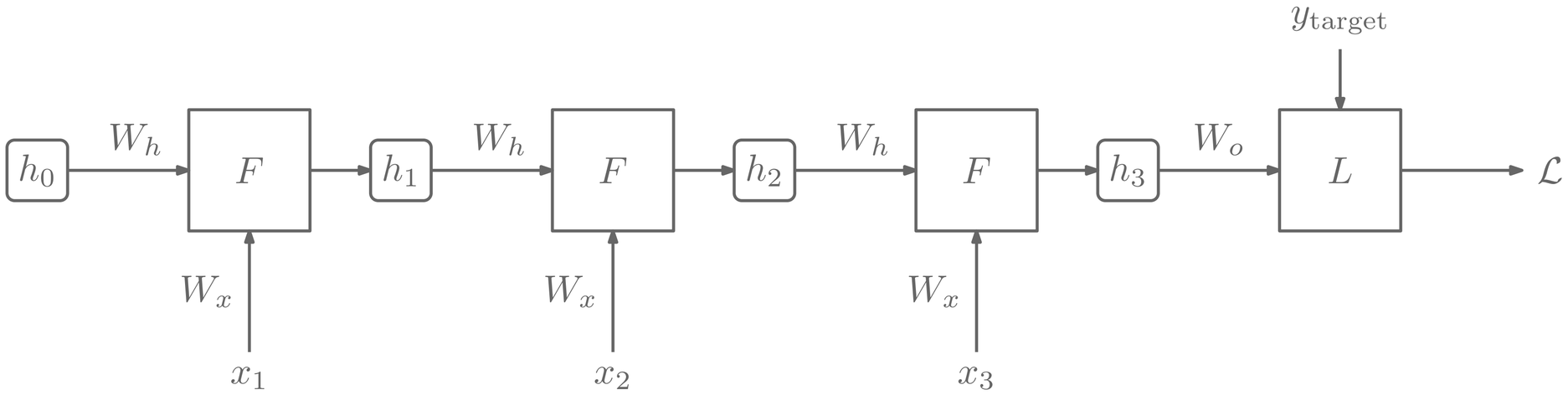
Exploding and vanishing gradients



- Computing the gradient we have, for example,

$$\frac{\partial \mathcal{L}}{\partial h_1} = \frac{\partial \mathcal{L}}{\partial y} \frac{\partial y}{\partial h_T} \frac{\partial h_T}{\partial h_{T-1}} \cdots \frac{\partial h_2}{\partial h_1}$$

Exploding and vanishing gradients

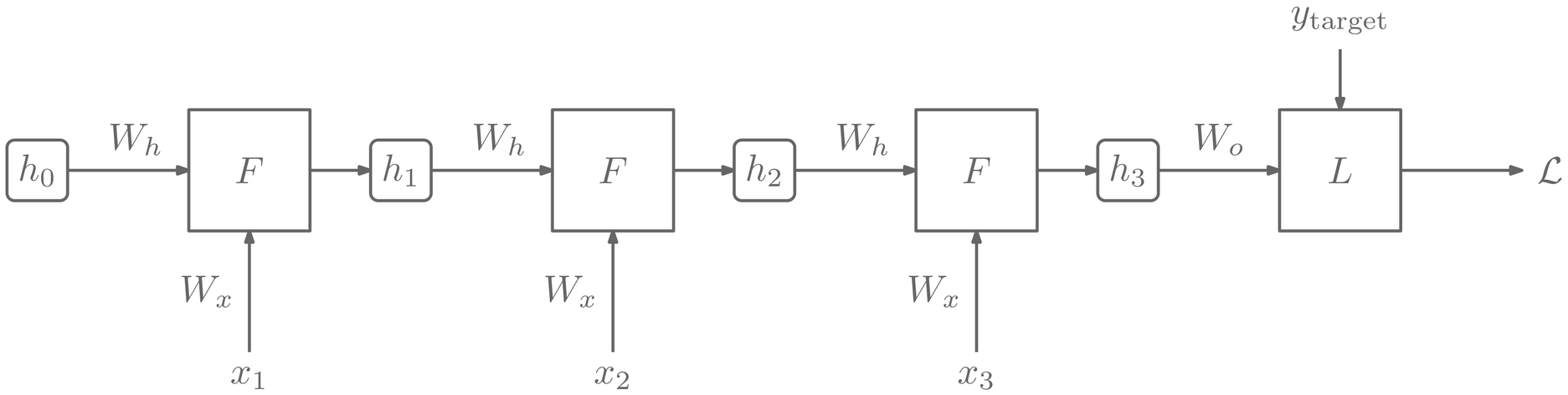


- Computing the gradient we have, for example,

$$\frac{\partial \mathcal{L}}{\partial h_1} = \frac{\partial \mathcal{L}}{\partial y}\frac{\partial y}{\partial h_T}\prod_{t=2}^{T}\frac{\partial h_t}{\partial h_{t-1}}$$

$$\frac{\partial h_t}{\partial h_{t-1}} = \text{diag}(F'(z_t))W_h$$

Exploding and vanishing gradients



- Computing the gradient we have, for example,

$$\frac{\partial \mathcal{L}}{\partial h_1} = \frac{\partial \mathcal{L}}{\partial y}\frac{\partial y}{\partial h_T}\prod_{t=2}^{T}\text{diag}(F'(z_t))W_h$$

Same matrix multiplied *T* times

Exploding and vanishing gradients

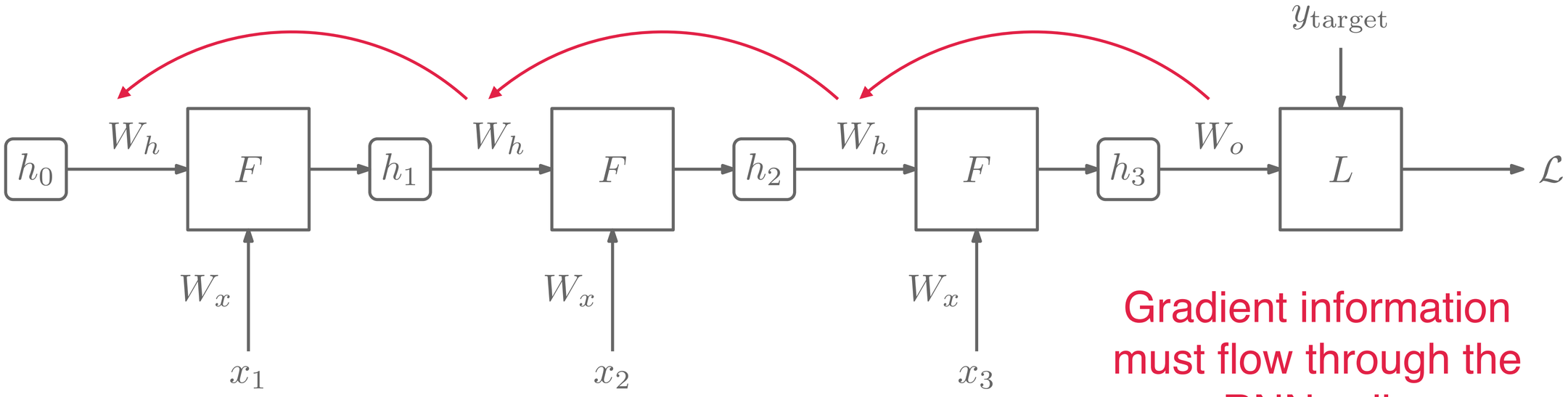
- Three cases:
  - If $\text{eig}(W_h) = 1$, gradient propagation is stable
  - If $\text{eig}(W_h) > 1$, gradient propagation explodes → Gradient clipping
  - If $\text{eig}(W_h) < 1$, gradient propagation vanishes
- Vanishing gradient is frequent and hard to deal with

Alternate RNN architectures

- Common approach to address vanishing gradients is to adopt alternative RNN architectures
  - Gated recurrent unit (GRU)
  - Long-short term memory (LSTM)

GRUs and LSTMs

The problem with the gradients

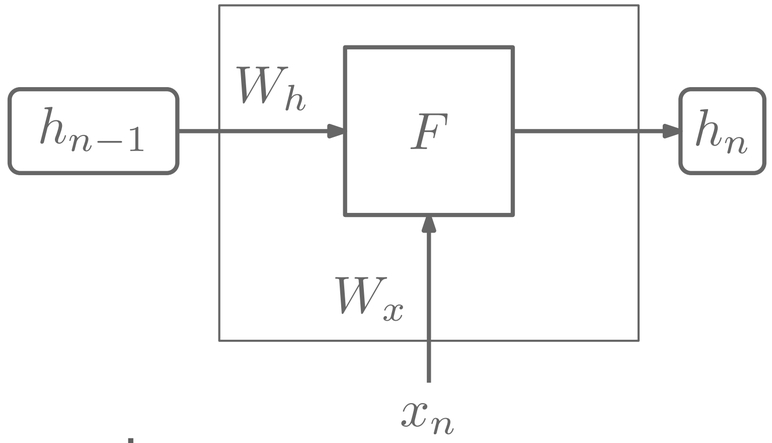


Gradient information must flow through the RNN cells

The problem with the gradients

- One possibility would be to add “short-circuits” to the network to facilitate the “flow” of gradient information

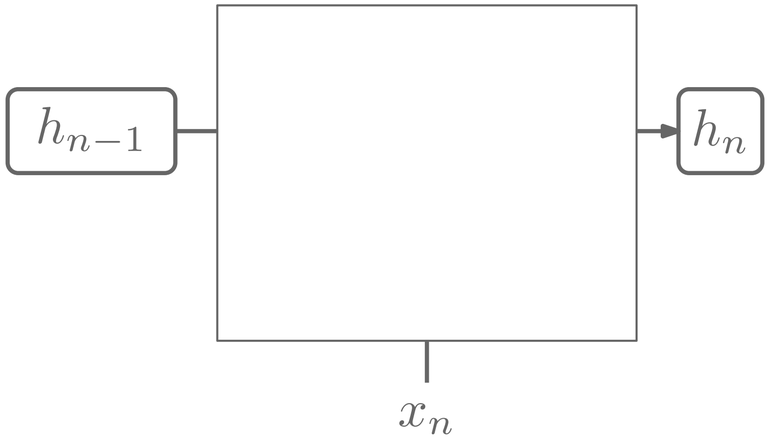
Recurrent Unit



- In a standard recurrent unit, we have:

$$h_n = F(W_x x_n + W_h h_{n-1})$$

Gated Recurrent Unit (GRU)

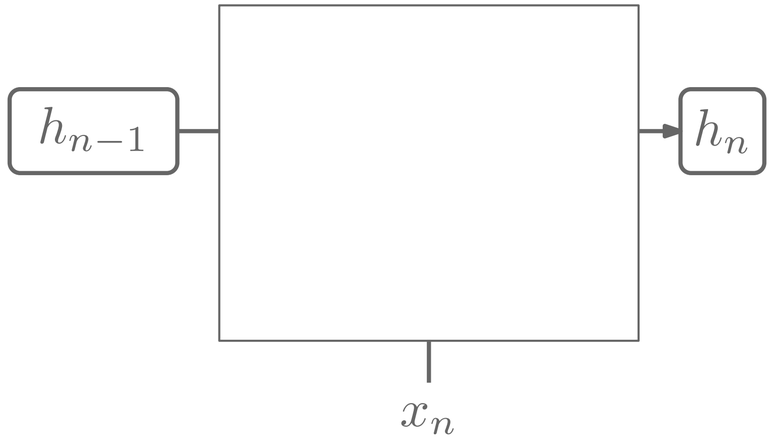


- Now…

$$h_n = F(W_x x_n + W_h h_{n-1})$$

Add a term that allows the unit to “forget”

Gated Recurrent Unit (GRU)



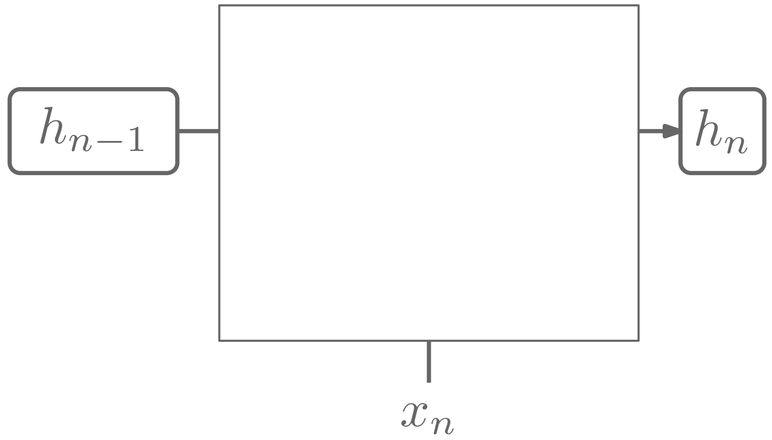
- Now…

$$\tilde{h}_n = F(W_x x_n + W_h(r_n \odot h_{n-1}))$$

Candidate internal state

Add a term that allows the unit to “forget”

Gated Recurrent Unit (GRU)



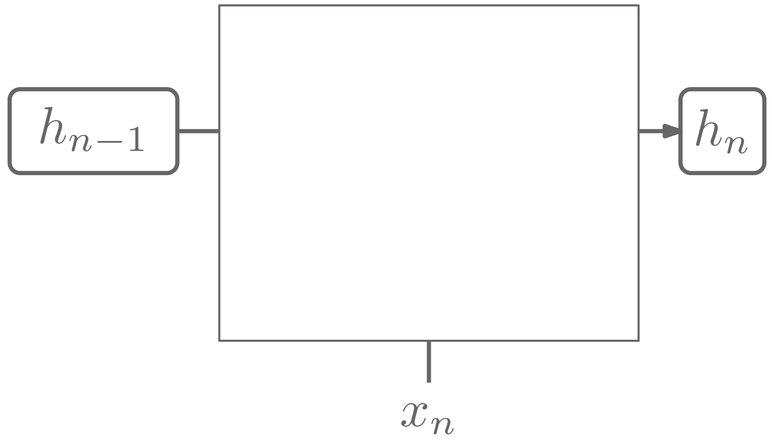
- Now…

$$\tilde{h}_n = F(W_x x_n + W_h(r_n \odot h_{n-1}))$$

$$h_n = u_n \odot \tilde{h}_n + (1 - u_n) \odot h_{n-1}$$

New internal state combines new candidate and old

Gated Recurrent Unit (GRU)

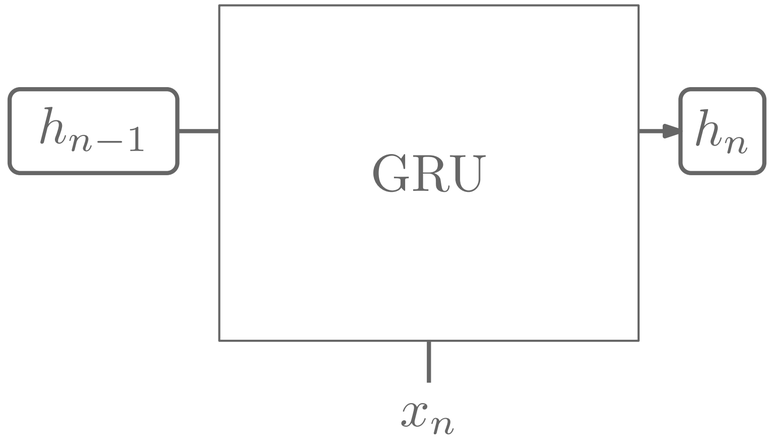


- Now…

$$\tilde{h}_n = F(W_x x_n + W_h(r_n \odot h_{n-1}))$$
$$h_n = u_n \odot \tilde{h}_n + (1 - u_n) \odot h_{n-1}$$
$$r_n = \sigma(W_{x,r} x_n + W_{h,r} h_{n-1})$$

Reset signal computed from current input and previous state

Gated Recurrent Unit (GRU)



- Now…

$$\tilde{h}_n = F(W_x x_n + W_h(r_n \odot h_{n-1}))$$

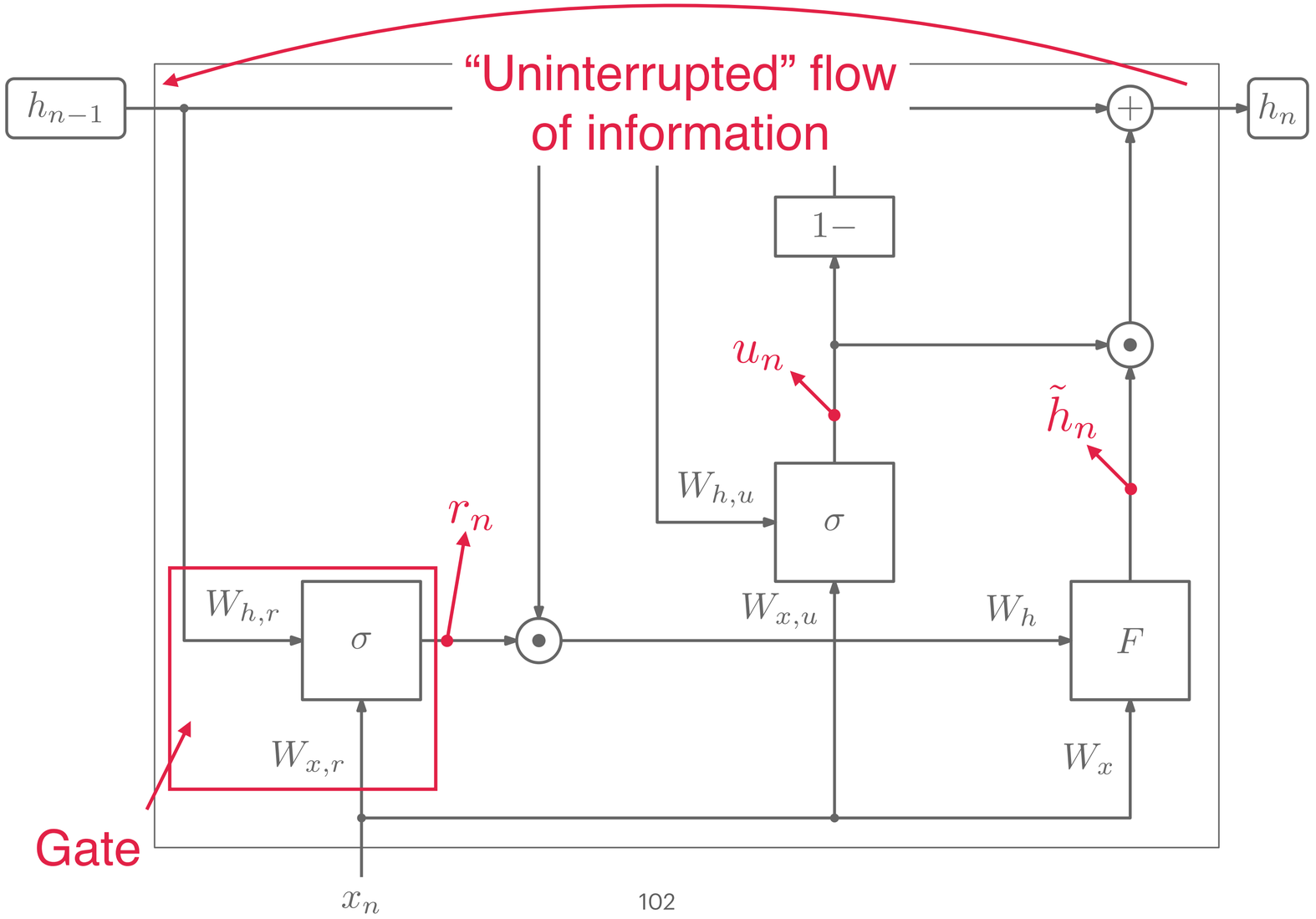
$$h_n = u_n \odot \tilde{h}_n + (1 - u_n) \odot h_{n-1}$$

$$r_n = \sigma(W_{x,r} x_n + W_{h,r} h_{n-1})$$

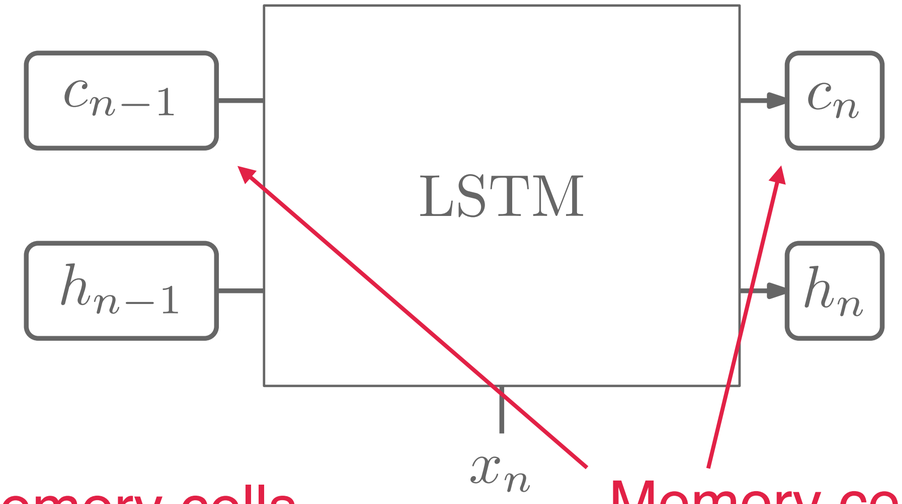
$$u_n = \sigma(W_{x,u} x_n + W_{h,u} h_{n-1})$$

Update signal computed from current input and previous state

Gated Recurrent Unit (GRU)



Long-Short Term Memory (LSTM)



- LSTM units also include memory cells
  - A second internal vector that is updated additively
  - Memory cells controlled through input, forget and output gates

Long-Short Term Memory (LSTM)

- In an LSTM,

$$\tilde{c}_n = F_c(W_{x,c}x_n + W_{h,c}h_{n-1})$$

Candidate
cell value

Long-Short Term Memory (LSTM)

- In an LSTM,

$$\tilde{c}_n = F_c(W_{x,c}x_n + W_{h,c}h_{n-1})$$
$$c_n = i_n \odot \tilde{c}_n + f_n \odot c_{n-1}$$

New cell value

Input gate (controls input of new information)

Forget gate (controls forgetting of old information)

Long-Short Term Memory (LSTM)

- In an LSTM,

$$\tilde{c}_n = F_c(W_{x,c}x_n + W_{h,c}h_{n-1})$$
$$c_n = i_n \odot \tilde{c}_n + f_n \odot c_{n-1}$$
$$h_n = o_n \odot F_h(c_n)$$

Internal state

Output gate (controls how much memory info goes out)

Long-Short Term Memory (LSTM)

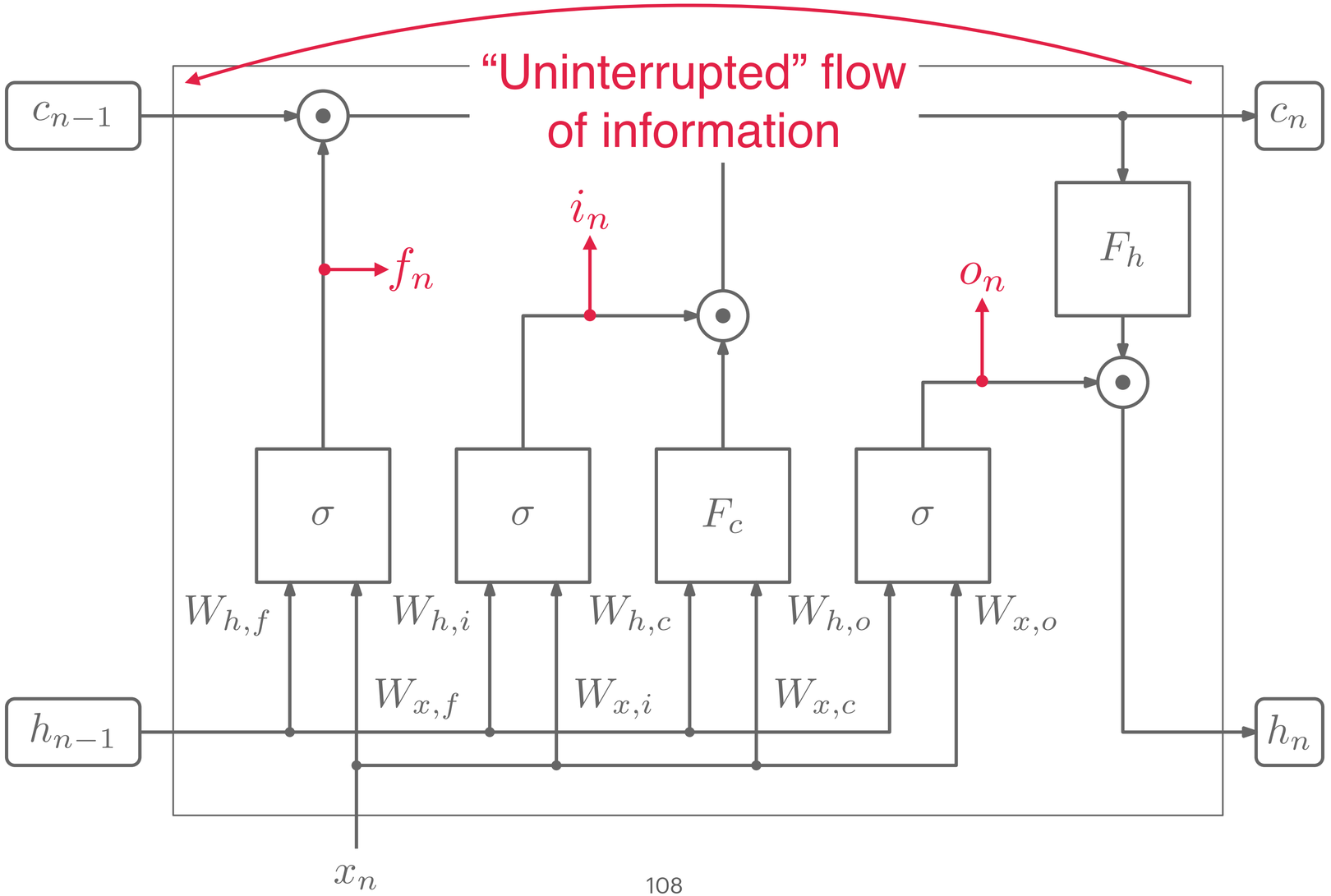
- In an LSTM,

$$\tilde{c}_n = F_c(W_{x,c}x_n + W_{h,c}h_{n-1})$$
$$c_n = i_n \odot \tilde{c}_n + f_n \odot c_{n-1}$$
$$h_n = o_n \odot F_h(c_n)$$

$$i_n = \sigma(W_{x,i}x_n + W_{h,i}h_{n-1})$$
$$f_n = \sigma(W_{x,f}x_n + W_{h,f}h_{n-1})$$
$$o_n = \sigma(W_{x,o}x_n + W_{h,o}h_{n-1})$$

Gates

Long-Short Term Memory (LSTM)

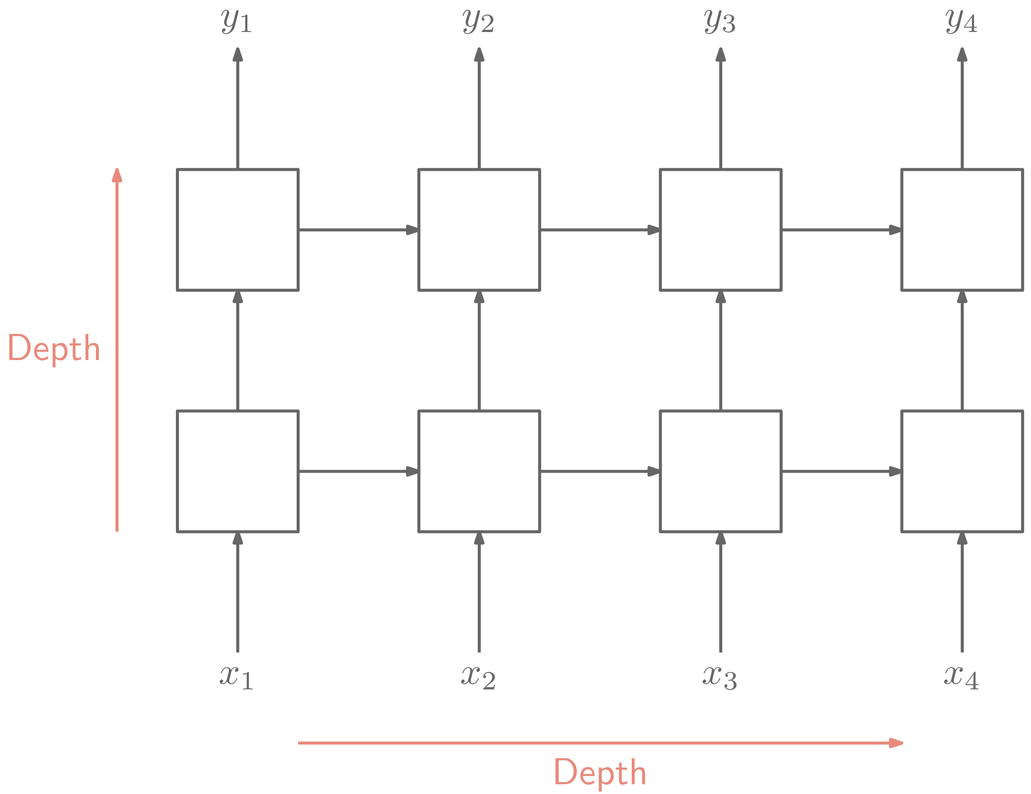


Final remarks

- LSTMs have better gradient propagation thanks to additive updates
- Variants exist that simplify some of the gates
- Have been used extensively in NLP tasks:
  - Named entity recognition
  - Machine translation
  - …

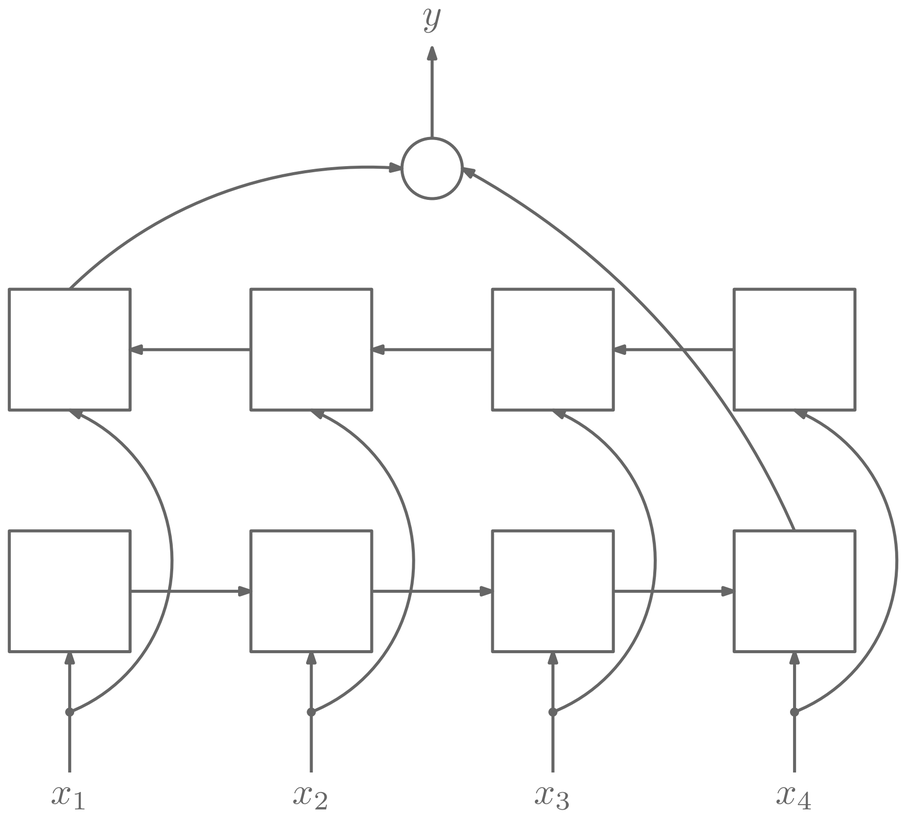
Final remarks

- Depth in recurrent layers helps (standard 2-8 recurrent layers)



Final remarks

- Bidirectional RNNs can be implemented with standard RNN cells, or GRUs or LSTMs



Final remarks

- Dropout can be added between layers, but not on recurrent connections
- For mini-batching, it is often necessary to pad the sequences to ensure constant length within the mini-batch

Summary

- Neural nets learn internal representations that can be transferred across tasks
- Distributed representations are exponentially more compact and allow generalizing to unseen objects
- Auto-encoders are an effective means for learning representations
- Word embeddings are continuous representations of words that are extremely useful in NLP

Summary

- Recurrent neural networks allow to take advantage of sequential input structure
- They can generate, tag, and classify sequences
- RNNs are trained with back-propagation through time
- Vanilla RNNs suffer from vanishing and exploding gradients
- LSTMs and other gated units are more complex RNNs that avoid vanishing gradients
- They can be extended to other structures like trees, images, and graphs

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